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SAM-CE: A THREE DIMENSIONAL MONTE CARLO CODE FOR THE SOLUTION OF THE FORWARD NEUTRON AND FORWARD AND ADJOINT GAMMA RAY TRANSPORT EQUATIONS - REVISION C

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20. ABSTRACT (Continue on reverse side if necessary and identify by block number)

The SAM-CE system is a FORTRAN Monte Carlo computer code designed to solve the time-dependent neutron and gamma ray transport equations in complex three-dimensional geometries.

SAM-CE is applicable for forward neutron calculations and for forward as well as adjoint primary gamma ray calculations. In addition, SAM-CE is applicable for the gamma ray stage of the coupled neutron-secondary gamma ray problem, which also may be solved in either the forward or the adjoint mode.

20. (continued)

Time-dependent fluxes, and flux functionals such as dose, heating, count rates, etc., are calculated as function of energy, time and position. Multiple scoring regions are permitted and these may be either finite volume regions or point detectors or both. Other scores of interest, e.g., collision and absorption densities, etc., are also made.

A special feature of SAM-CE is its use of the "combinatorial geometry" technique which affords the user geometric capabilities exceeding those available with other commonly used geometric packages. An automatic geometry checker is included.

All nuclear interaction cross section data (derived from the ENDF IV libraries) are tabulated in point energy meshes. The energy meshes for neutrons are internally derived, based on built-in convergence criteria and user-supplied tolerances. Tabulated neutron data for each distinct nuclide are in unique and appropriate energy meshes. Both resolved and unresolved resonance parameters from ENDF data files are treated automatically and extremely precise and detailed descriptions of cross section behavior is permitted. Such treatment avoids the ambiguities usually associated with multi-group codes, which use flux-averaged cross sections based on assumed flux distributions which may not be appropriate.

By use of the "band" feature of the code, which automatically splits cross section data into two or more energy ranges to be treated one at a time, SAM-CE affords one the ability to consider many nuclides, in a given configuration, each being described in much detail.

SAM-CE also provides the user with the opportunity to employ energy, region and angular importance sampling.

An extensive library of processed cross sections for use in SAM-CE is available at the Radiation Shielding Information Center (RSIC), ORNL, Oak Ridge, Tennessee.

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1.1 General Description of the SAM-CE System

The SAM-CE system is a FORTRAN Monte Carlo computer code designed to solve the time-dependent neutron and gamma ray transport equations in complex three-dimensional geometries.

SAM-CE is applicable for forward neutron calculations and for forward as well as adjoint primary gamma ray calculations. In addition, SAM-CE is applicable for the gamma ray stage of the coupled neutron-secondary gamma ray problem, which also may be solved in either the forward or the adjoint mode.

Time-dependent fluxes, and flux functionals such as dose, heating, count rates, etc., are calculated as functions of energy, time and position. Multiple scoring regions are permitted and these may be either finite volume regions or point detectors or both. Scores at point detectors are made by a new "bounded-estimator" procedure which completely eliminates the possibility of "blow-up" scores due to the usual inverse-square estimation process. Other scores of interest, e.g., collision density and energy deposition, are also made.

A special feature of SAM-CE is its use of the "Combinatorial Geometry" technique which affords the user geometric capabilities exceeding those available with other commonly used geometric packages. Sophisticated procedures have been built into the code to allow the user, as an option, to check automatically the validity of the geometry input data.

All neutron and gamma ray cross section data, as well as gamma ray production data, are derived from the ENDF libraries,[1] and are tabulated in point energy meshes. These energy meshes are internally derived, and are based on built-in convergence

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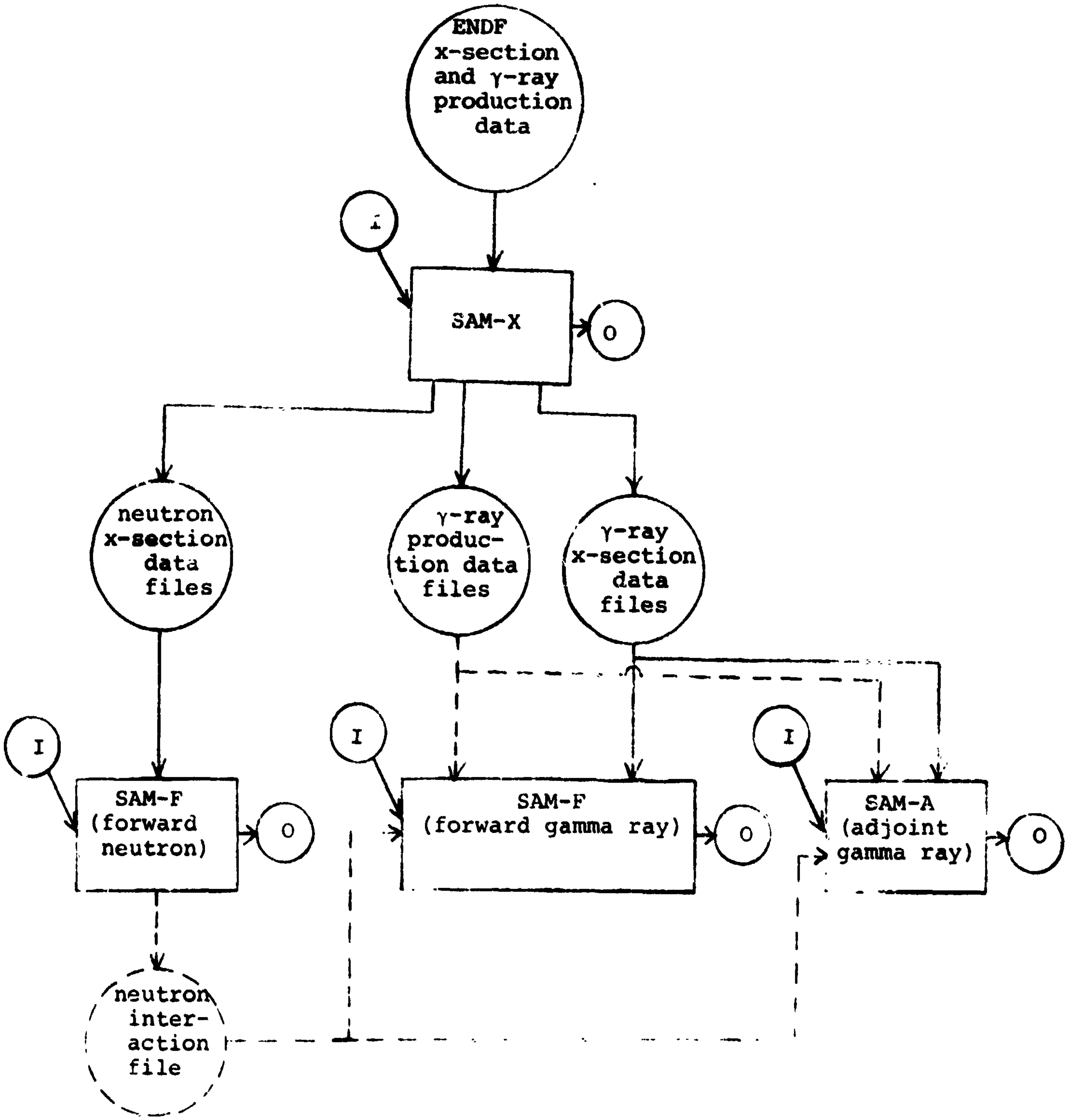
criteria, which, as an option, may be overridden by the user. Tabulated data for each distinct nuclide are thus in unique and appropriate energy meshes. Both resolved and unresolved resonance parameters from ENDF neutron data files are treated automatically and extremely precise and detailed descriptions of cross section behavior is permitted. Such treatment avoids the ambiguities usually associated with multi-group codes, which use flux-averaged cross sections based on assumed flux distributions which may or may not be appropriate.

By use of the special "band" feature of the code, which automatically splits cross section data into two or more energy ranges to be treated one at a time, SAM-CE affords one the ability to consider many nuclides, in a given configuration, each being described in much detail.

SAM-CE also provides the user with the opportunity to employ energy, region and angular importance sampling. Also, thermal neutron (Maxwellian-averaged) cross section treatment and a thermal neutron diffusion options are available for low energy neutron problems.

1.2 Organization of the SAM-CE System

SAM-CE is a system composed of three separate programs; SAM-F and SAM-A for forward and adjoint Monte Carlo calculations, respectively, and SAM-X, a pre-processor for neutron and gamma ray cross section as well as for gamma ray production data. The overall organization of the SAM-CE system is outlined in Figure 1.1.



NOTE: I = Input Data
O = Edited Output
Dashed lines are for secondary γ-ray problems only.

Figure 1.1 SAM-CE System

Consider first the use of SAM-X. Neutron and gamma ray cross section and gamma ray production data, in the form of files from an ENDF library,* are supplied to program. For the user-specified materials, SAM-X extracts the necessary raw information and organizes the data into the format required by the SAM-F and SAM-A Monte Carlo codes. If neutron resonance parameters are supplied by ENDF, SAM-X will reconstruct point energy cross section values in the resonance range in an appropriate internally-determined energy mesh. The output files of SAM-X are processed neutron and gamma ray cross section and gamma ray production data tapes which, in general, are saved and thus need not be recreated until the basic ENDF library itself is revised for one or more nuclides of interest. At that time, only the revised nuclides need be reprocessed.

Next in sequence is SAM-F, the forward Monte Carlo program. SAM-F, (consider first the neutron case) reads in the neutron cross section data, generated by SAM-X, and geometry and other descriptive data supplied as input. The neutron source may be either generated internally from input provided by the user or may be supplied in the form of a previously created "external" source tape. The latter may be generated by any user-developed ad hoc coding providing the output is in the specified format.

SAM-F then calculates and provides an edit of the desired neutron fluxes and flux-functionals. In addition, if either a forward <u>or</u> adjoint secondary gamma ray problem is to follow the neutron calculation, the output will also consist of a neutron "interaction" tape. This tape contains records of all the inter-

* Also referred to in the literature as "ENDF/B."

action experienced by neutrons, in the Monte Carlo game just completed, which could possibly lead to the production of secondary gamma radiation. Subsequently, the interaction tape is read into either program SAM-F (gamma ray mode) or SAM-A. These codes use the nuclide tables of gamma ray production data, generated by SAM-X, to convert the interaction data into a secondary gamma ray source.

Consider next gamma ray transport. Either SAM-F (forward) or SAM-A (adjoint) may be used. In general, a small source and a distributed scoring region situation is amenable to solution by forward Monte Carlo -- thus SAM-F. Conversely, a distributed source and a point scoring region situation lends itself well to solution by adjoint Monte Carlo -- thus, SAM-A.* Note that since secondary gamma ray problems almost always involve distributed sources of the secondary radiation, SAM-A is often used in this situation. The commonly encountered point neutron source - point secondary gamma ray detector configuration is examined efficiently by use of SAM-F for neutrons and SAM-A for secondary gamma radiation.

For gamma ray transport, as was the case for neutron transport, the source may be either internally generated or supplied as an external source tape.** In addition, the neutron interaction tape described above may be used in lieu of a source description.

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* At present, SAM-A detector regions must be point detectors, or one of the simple geometric bodies of the Combinatorial Geometry package.

** At present, SAM-A cannot generate primary sources internally. It can, however, be used to link up with an arbitrary surrounding surface and thus can be used as a "vulnerability-type" code.

Using these data and geometry and other input descriptions provided by the user, both SAM-F and SAM-A calculate and provide edits of the desired (primary or secondary) gamma ray fluxes and flux functionals.

1.3 Organization of this SAM-CE Manual

Sections 2, 3 and 4, which follow, describe in detail the SAM-X, SAM-F and SAM-A programs, respectively. Descriptions of input and output as well as tape and disk file assignments are provided.

SECTION 2 - PROGRAM SAM-X

2.1 General Description of the SAM-X Program

With the establishment of the Cross Section Evaluation Center at Brookhaven National Laboratory, detailed and up-to-date evaluated cross section information, in the form of the ENDF files, has become available. In order to make use of this wealth of accurate information in the SAM-CE System, the SAM-X program which generates processed cross section data tapes for later use in the SAM-F and SAM-A Monte Carlo codes, was written.

SAM-X is designed to process ENDF neutron and gamma ray cross section and gamma ray production data files. The output of SAM-X is a neutron element data tape (NEDT)*, a gamma ray production data tape (GPDT)*, and a gamma ray element data tape (GEDT)*, which are subsequently used as input to the SAM-F and SAM-A Monte Carlo transport codes.

SAM-X is a program with an overlay structure. The code comprises a small driver (main overlay), and five processors (primary overlays): NUTRON, PEND, WEED, GAMMA and BCDEAN.** Program NUTRON processes the ENDF neutron files. Program PEND (Production from Evaluated Nuclear Data) processes the ENDF photon production files. Program WEED (Weed-out Extra Energy-dependent Data), which complements PEND, is a data reduction code. Program GAMMA processes the ENDF gamma ray cross section files. Program BCDEAN convects the normal binary mode output of SAM-X to BCD mode for inter-facility

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* In the descriptions that follow, EDT (element data tape) will generally refer to either an NEDT, a GPDT, or a GEDT, where the specific reference intended is clear from context.

** Referred to as NUTRON, PEND, WEED, GAMMA and BCDEAN throughout Section 2, these primary overlay programs are actually coded as PROGRAM OVER10, OVER20, OVER30, OVER40 and OVER50, respectively, as convenient flags in switching from CDC to IBM versions.

transmission of processed data.*

NUTRON reads the ENDF neutron files (File 1 through 5) and calculates total, total scattering, and inelastic cross sections and establishes the tables required to treat the angular distribution of neutrons emerging from scattering collisions and the energy distribution of those emerging from inelastic scattering collisions. The code permits Doppler broadening in the resolved resonance range.**

The organization of an NEDT for an element is given in Appendix A.

Program PEND reads the ENDF photon production files (File 12 through File 15) and the related neutron files (File 1 and File 3). The code processes this ENDF information and produces a gamma production data tape (GPDT) to be used as input for SAM-F and SAM-A for the solution of forward and adjoint secondary gamma ray transport problems. The organization of a GPDT for an element is described in Appendix D. It should be noted that the code treats anisotropy of gamma ray production - provided such information is given by ENDF in File 14.

The potentially large GPDT, which may be produced for one element by PEND, motivated the development of the data reduction program, WEED. This overlay of SAM-X is designed to reduce the size of a GPDT. Normally, the original GPDT produced by PEND is processed by WEED with default criteria governing the extent of the

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* BCDEAN can also operate as a stand alone code and convert BCD mode data to binary mode on either an IBM or CDC machine.

**In the present version, no attempt has been made to extend the treatment to all energies since the effect has little significance in shielding calculations.

data reduction. But WEED may be utilized to reprocess a GPDT which has already been "WEED-ed", if so required. In addition, the internally set default criteria may be superseded by user-specified criteria.

Program GAMMA reads the ENDF gamma ray cross section file (File 23). Since both Monte Carlo codes, SAM-F and SAM-A, do not consider coherent scattering at the present time, the total cross sections (MT=501) given by ENDF are modified by subtracting out the coherent scattering (MT=502). GAMMA then treats incoherent scattering (MT=504) and re-tabulates it in the same energy mesh as the modified total cross sections. Note that the Monte Carlo programs subsequently use the classic Klein-Nishina distribution for scattering so that an inconsistency develops in the low energy (x-ray) range.* The organization of a GEDT for an element is described in Appendix B.

The machine dependence of the binary EDT produced by the first four primary overlays motivated the development of the post processing program, BCDEAN. This fifth primary overlay serves as a two way EDT converter, i.e., binary-to-BCD and vice versa. The structure of a typical BCD EDT is described in Appendix N.

The user may now proceed to Section 2.5, 2.6 and 2.7 which contain descriptions of the input, additional notes to the user, and tape and file utilization, respectively. However, those desiring a more thorough background of SAM-X may wish to read Section 2.2, 2.3 and 2.4 which contain a general description of the ENDF System, the theory behind the SAM-X code, and the program information flow, respectively.

* Development is currently underway to provide SAM-CE with rigorous x-ray cross section treatment. This full x-ray capability will be available in 1975, upon the issuance of the next official revision to the code.

2.2 ENDF (Evaluated Nuclear Data File) System*

The structure of the magnetic tape containing the ENDF data, consisting of BCD card images as required by SAM-X, is shown in Figure 2.1. A single record written at the beginning of the tape serves as identification, and a single record written at the end signals the end of the tape. Between these records, information is subdivided into data for given materials (labeled MAT). The data for a particular material are divided further into files (labeled MF), each containing certain classes of information. A file is subdivided into sections (labeled MT), corresponding to data for a particular type of reaction. For convenience, Files 1 through 7 may be referred to as the neutron files, Files 12 through 15 as the photon production files, and File 23 as the gamma ray cross section file.

For a given material, File 1 (general information) consists of one or more sections containing a Hollerith description of the material, a "dictionary" of the data to follow, and data relating to the number of neutrons produced per fission, to decay, and to fission product yields. File 2 consists of one section containing parameters for resolved and unresolved resonances. Cross sections computed from the parameters in this file, (if any), are added to the "smooth" cross sections given in File 3, consisting of one section for each tabulated reaction type. Secondary angular and energy distributions, expressed as normalized probability distributions, are given in Files 4 and 5, respectively, with one section corresponding to each reaction type represented. Files 6 and 7 contain data related to correlated angle and energy distributions of

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* Also referred to in the literature as ENDF/B.

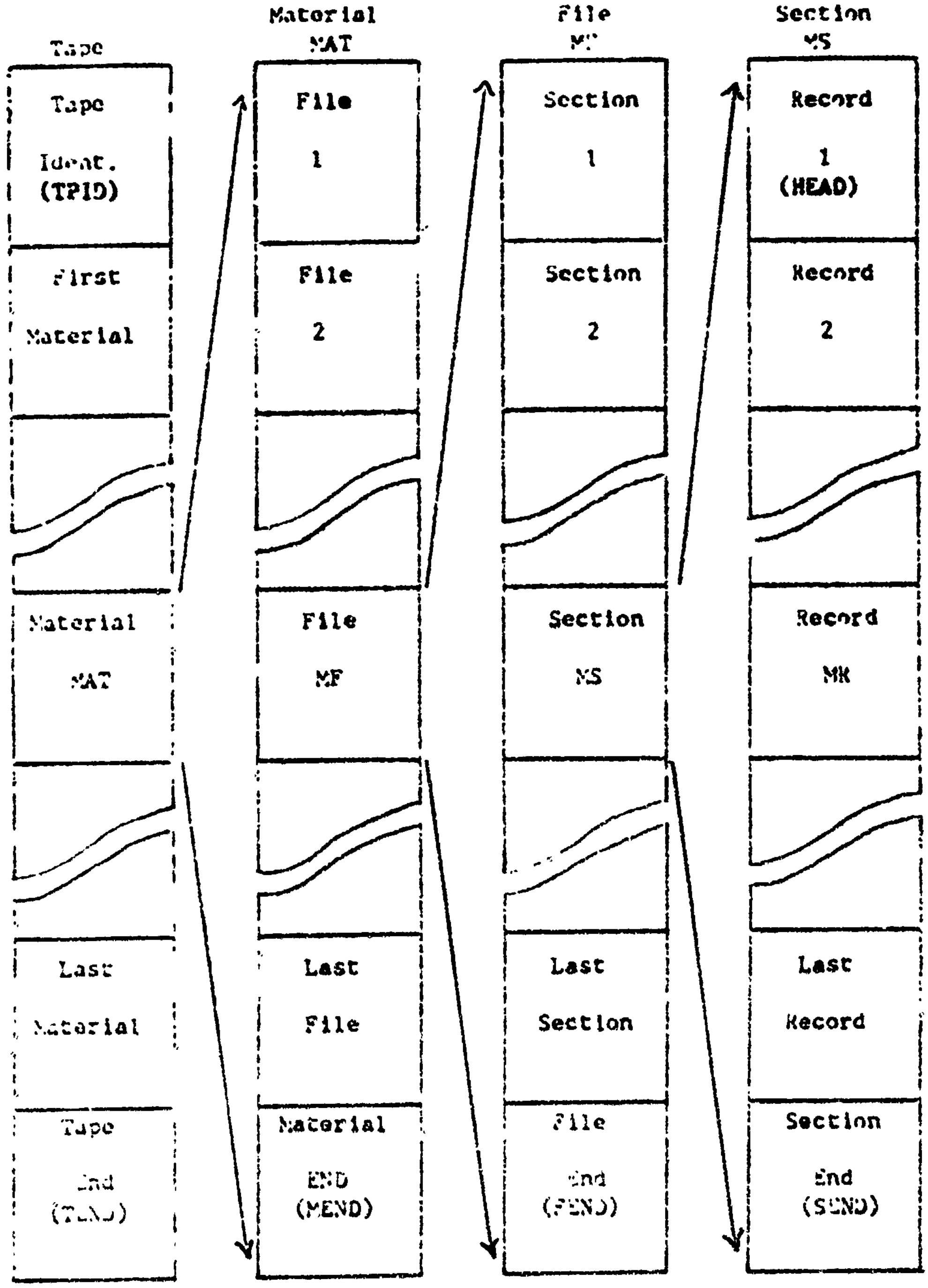

Figure 2.1 - Arrangement of an ENDF Tape

secondary neutrons, and to thermal scattering laws, respectively, but are not utilized in the present version of the SAM-X program.

A description of the formats for photon production data is given by Dudziak[2]. As is the case for the neutron data, the photon production data for a given material are divided into files, each containing certain classes of data. A file is subdivided into sections, each containing data for a particular reaction. These reaction types are designated by the same set of MT numbers which were assigned for the neutron files. Finally, for photon production data, a section is divided into subsections, one for each discrete photon and one for the continuum, if any.

In FILE 12, under option LO=1, tabulations of multiplicities, or partial photon yields, are given corresponding to incident neutron energies. This file has no analog in the neutron files.

The structure of FILE 13 parallels that of FILE 12, except that its subsections are tabulations of the photon production cross sections. Photon production FILE 13 is analogous to the neutron FILE 3 (Smooth Cross Sections).

Photon angular distributions appear in File 14. The LI option serves to flag isotropic distributions (LI=1). Anisotropy for some photons is signaled by LI=0, and LTT=1 or 2, for Legendre coefficients or tabulated representation, respectively. Photon production FILE 14 is analogous to neutron FILE 4.

Normalized energy distributions of continuous photon spectra are the only data given in FILE 15. The system is identical to that used in the corresponding neutron FILE 5 (Secondary Energy Distribution) except that, at present, the only continuous distribution law activated is an arbitrary tabulated function, flagged by LF=1.

Photon cross sections appear in FILE 23. Note that SAM-X subtracts out the coherent scattering cross sections (MT=502) from the total cross section (MT=501) since coherent scattering is not treated, at the present time, by either SAM-F or SAM-A.

2.3 SAM-X Program - Theory

2.3.1 Treatment of the Resonance Region

The data may be given for individual isotopes in a material. For each isotope, the data may be subdivided into energy ranges in each of which a different representation is employed. It is assumed by the code that ranges, given in order of increasing energy, do not overlap. Generally, two energy ranges are used to describe resolved and unresolved resonances, respectively.

2.3.1.1 Resolved Resonance Region

SAM-X utilizes resolved parameters, depending on both ℓ (orbital) and J (total) angular momentum in the single-level Breit-Wigner formula with interference, as described in Appendix D of Reference 1. The formulas appearing in Gregson et al.[4] omitting the resonance-resonance interference term have been adopted. Written in the laboratory system without Doppler broadening for a given ℓ and for the isotope m, the cross sections are expressed as:

Elastic Scattering Cross Section

$$\sigma_{nn}(E) = \sum_{\ell=0}^{NLS} \sigma_{nn}^{\ell}(E), \text{ where}$$

$$\sigma_{nn}^{\ell}(m) = (2\ell+1)\cdot\frac{4\pi}{k_m^2}\cdot\sin^2\phi_\ell$$

$$+ \frac{\pi}{k_m^2}\sum_J g_J \sum_{r=1}^{N_r(\ell,J)}\left[\frac{\Gamma_{nr}^2\cos 2\phi_\ell - 2\Gamma_{nr}(\Gamma_{\gamma r}+\Gamma_{fr})\sin^2\phi_\ell + 2(E-E_r')\Gamma_{nr}\sin 2\phi_\ell}{(E-E_r')^2+\Gamma_r^2/4}\right]$$

$$+ \frac{\pi}{k_m^2}\sum_J g_J \sum_{r=2}^{N_r(\ell,J)} \sum_{s=1}^{r-1} \frac{2\Gamma_{nr}\Gamma_{ns}\left[(E-E_r')(E-E_s') + \frac{1}{4}\Gamma_r\Gamma_s\right]}{\left[(E-E_r')^2 + \frac{1}{4}\Gamma_r^2\right]\left[(E-E_s')^2 + \frac{1}{4}\Gamma_s^2\right]}. \qquad (1)$$

Radiative Capture Cross Section

$$\sigma_{n\gamma}(E) = \sum_{\ell=0}^{NLS} \sigma_{n\gamma}^{\ell}(E), \text{ where}$$

$$\sigma_{n\gamma}^{\ell}(m) = \frac{\pi}{k_m^2}\sum_J g_J \sum_{r=1}^{N_r(\ell,J)} \frac{\Gamma_{nr}\Gamma_{\gamma r}}{(E-E_r')^2+\Gamma_r^2/4} \qquad (2)$$

Fission Cross Section

$$\sigma_{nf}(E) = \sum_{\ell=0}^{NLS} \sigma_{nf}^{\ell}(E), \text{ where}$$

$$\sigma_{nf}^{\ell}(m) = \frac{\pi}{k_m^2}\sum_J g_J \sum_{r=1}^{N_r(\ell,J)} \frac{\Gamma_{nr}\Gamma_{fr}}{(E-E_r')^2+\Gamma_r^2/4} \qquad (3)$$

where NLS is given in File 2 for each isotope and $g_J = (2J+1)/2(2I+1)$. I is the spin of the target nucleus and J is the spin of the compound nucleus for the resonance state.

The sums over J in Eqs. 1 through 3 extend over the $N_J(\ell)$ possible values of the angular momentum of the resonant states of the compound nucleus excited by the incident partial wave ℓ. The sums over r extend over the number of resonances $N_r(\ell,J)$ for each pair of values of ℓ and J. The following quantities are defined:

$$\Gamma_{nr}(E) = \text{neutron width} = \frac{P_\ell(E)\Gamma_{nr}(|E_r|)}{P_\ell(|E_r|)}$$

$$\Gamma_r(E) = \text{total width} = \Gamma_{nr}(E) + \Gamma_{\gamma r} + \Gamma_{fr}$$

$$E_r' = E_r + \left[\frac{S_\ell(|E_r|) - S_\ell(E)}{2P_\ell(|E_r|)}\right] \Gamma_{nr}(|E_r|)$$

E_r = energy, in ev, of the peak of resonance r*

E = neutron energy, in ev, in the laboratory system

k_m = neutron wave number in the center-of-mass system

$=2.196771 \times 10^{-3} \left(\frac{A}{A+1}\right) \sqrt{E}\ (\text{barns})^{-\frac{1}{2}}$

A = ratio of the atomic weight of isotope m in the ($C^{12} = 12$) scale to that of the neutron.

Formulas for the shift factor, S_ℓ, penetration factor, P_ℓ, and phase shift, ϕ_ℓ, are given in Table 2.1 for values of ℓ from 0 to 3, the maximum permitted by the SAM-X program.

Cross sections are calculated on an energy mesh with the density of points determined so that linear interpolation will yield

* For bound levels, the absolute value, $|E_r|$, is used.

TABLE 2.1-FORMULAS FOR THE SHIFT FACTOR, PENETRATION FACTOR, AND PHASE SHIFT FOR VALUES OF ℓ FROM 0 TO 3

Orbital Momentum, ℓ	Shift Factor, S_ℓ	Penetration Factor, P_ℓ	Phase Shift, φ_ℓ
0	0	ρ	ρ
1	$-\frac{1}{1+\rho^2}$	$\frac{\rho^3}{1+\rho^2}$	$\rho - \tan^{-1}\rho$
2	$-\frac{18+3\rho^2}{9+3\rho^2+\rho^4}$	$\frac{\rho^5}{9+3\rho^2+\rho^4}$	$\rho - \tan^{-1}\left(\frac{3\rho}{3-\rho^2}\right)$
3	$-\frac{675+90\rho^2+6\rho^4}{225+45\rho^2+6\rho^4+\rho^6}$	$\frac{\rho^7}{225+45\rho^2+6\rho^4+\rho^6}$	$\rho - \tan^{-1}\left(\frac{15\rho-\rho^3}{15-6\rho^2}\right)$

where $\rho = ka$

k = neutron wave number

a = channel radius.

reasonably accurate cross sections at output energies. An energy array is set up with end points equal to the end points of the output energy table, and intermediate points at each resonance peak. At each of these points the cross sections are computed by use of the formulas given above. If the energy at which the cross section is being calculated lies within a given number of widths of a specific resonance, that resonance is included in the sum over r in the formulas. The given number of widths, WIDTHS, is entered as input.

For each interval in the energy array established, starting at the low end, the integral over energy of either the absorption cross section or the total cross section is computed by use of the Trapezoidal Rule. Then the interval is subdivided by insertion of a midpoint, and the integration repeated for the pair of intervals. The sum of the integrals over the two halves is compared with that of the whole; if these quantities do not agree within an input criterion, EPS, the midpoint energy is added to the output table; if the integrals do agree, the next higher interval is treated.

The coding exists for Doppler broadening the resonances by multiplying the resonance terms by ψ and the interference term by χ, where ψ and χ are the line shape functions calculated in subroutine W, as written by O'Shea and Thacher.[5] However, when multilevel interference occurs no Doppler broadening is calculated by the code. Furthermore, no treatment of temperature dependence exists outside of the resolved resonance range. In practice, problems have been run in which the resonances have been Doppler-broadened at room temperature and added to the smooth cross sections of File 3, usually generated at that temperature.

2.3.1.2 Unresolved Resonance Range

The present requirements of the ENDF libraries have made desirable the use of a newly developed method for generation of cross sections in the unresolved resonance range. This method, (Gaussian Quadrature), has been placed into the code as the default (normal mode) option. The method of the MC^2 code[6], has been retained as an alternative option.

The method of the MC^2 code, which has been widely used to obtain average cross sections, is efficient for calculation when fluctuations are allowed in one or two of the resonance partial widths. However, the general case, now allowed by the ENDF, may involve concurrent resonance fluctuations in any or all of four partial widths, i.e., neutron, fission, radiative and competitive reaction widths. The fluctuating widths are each assumed to be picked from a separate and independent chi-square distribution with some number of degrees of freedom. This leads to the possibility of integration in up to four dimensions to obtain the average cross section. The method of MC^2 applied to three and four dimensional integration involves calculation at an excessive number of points. Furthermore, the weight constants utilized in the MC^2 method are not presently available for all cases of interest in the general multidimensional situation. The new calculational

approach (described below) avoids these difficulties by mathematically reducing the general multidimensional integral to integration in a single dimension. The remaining integration is accomplished by a Gaussian quadrature technique.

In both methods effective resonance cross sections are evaluated at discrete energy points, E*, established at equal lethargy intervals of width determined by input quantity DELU. The effective unresolved resonance capture cross section at E* is based on the expression:

$$\overline{\sigma_c(E^*)} = \frac{1}{E_2-E_1} \int_{E_1}^{E_2} \sum_s \sum_i \sigma_{c_i}^s(E)\,dE \qquad (4)$$

where energy limits E_1 and E_2 bound a small subinterval surrounding E*. The sum over s represents the sum over sequences of resonances, i.e., over particular values of angular momentum, ℓ, and channel spin, J; the sum over i represents the sum over resonances in a given sequence.

As described in Reference 6, the interval E_2-E_1 may be replaced by the average spacing of the resonances of sequence s, $\langle D^s \rangle$ times the number of resonances, N^s, contained in the interval. Since narrow resonances have been assumed, the integration limits may be changed from (E_1,E_2) to $(-\infty,\infty)$. Also, if the number of resonances in the interval is large, the sum over i may be replaced by an

integration over the neutron and fission width distribution $S_j(r)$ expressed as chi-squared distributions with j degrees of freedom, i.e.,

$$S_j(r)\,dr = \frac{j}{2}\,\frac{1}{\Gamma(j/2)}\left(\frac{jr}{2}\right)^{j/2-1} e^{-jr/2}dr \qquad (5)$$

where $r = \Gamma_n(E)/\overline{\Gamma_n(E^*)}$ is the ratio of neutron width at E to the mean neutron width at E*. Thus, Eq. 4 for nonfissile materials and zero competitive reaction width may be written as:

$$\overline{\sigma_c(E^*)} = \sum_s \frac{2\pi^2}{k^{*2}}\,\frac{g^s\,\overline{\Gamma_n^s(E^*)}\,\Gamma_\gamma^s}{\langle D^s\rangle}\int_0^\infty \frac{S_j(r)\,r\,dr}{\Gamma_\gamma^s + r\,\Gamma_n^s(E^*)} \qquad (6)$$

where the mean neutron width at E* for angular momentum ℓ and total channel spin J of a particular sequence s is given by the expression

$$\overline{\Gamma_n^s(E^*)_{\ell,J}} = \overline{\Gamma^o_{n_{\ell,J}}}\cdot\frac{\sqrt{E^*}\,P_\ell(E^*)\,\mu_{\ell,J}}{\rho^*}\ ;\ \rho^* = k^*a \qquad (7)$$

The reduced neutron width, $\Gamma^o_{n_{\ell,J}}$, and the number of degrees of freedom, $\mu_{\ell,J}$, are given on the ENDF data tape.

It is important to note throughout this discussion that any temperature dependence has been lost by use of the assumptions described above.

a) <u>Gaussian Quadrature Method (Default Option)</u>

The generation of Eq. 6 to include resonance fluctuations in any or all of the four partial widths is given as

$$\overline{\sigma_{n,i}(E^*)} = \sum_s \frac{2\pi^2}{K^{*2}} \frac{g^s}{\langle D^s \rangle} \left\langle \frac{\Gamma_n^s \Gamma_i^s}{\Gamma^s} \right\rangle \tag{8}$$

where

$$\Gamma_i^s = \Gamma_n^s, \Gamma_\gamma^s, \Gamma_f^s, \Gamma_x^s. \tag{9}$$

Γ_x^s is the competition reaction width. Also,

$$\Gamma^s = \Gamma_n^s + \Gamma_\gamma^s + \Gamma_f^s + \Gamma_x^s \tag{10}$$

and for fluctuating widths,

$$\Gamma_i^s = \overline{\Gamma}_i^s r_i \tag{11}$$

The variable r_i follows the chi-squared distribution with ν_i degrees of freedom. It is then shown in Appendix M that,

$$\left\langle \frac{\Gamma_n^s \Gamma_i^s}{\Gamma_s} \right\rangle = \frac{\overline{\Gamma}_n^s \overline{\Gamma}_i^s}{\overline{\Gamma}^s \nu_n \nu_i} \prod_{i=1}^{n} 2^{m_i} \Gamma(m_i+\nu_i/2)/\Gamma(\nu_i/2) H, \tag{12}$$

$$H = 2 \int_{-1}^{+1} (1+\mu)^{-2} \prod_{i=1}^{n} \left[1 + \frac{2\overline{\Gamma}_i^s}{\nu_i \overline{\Gamma}^s} \frac{1-\mu}{1+\mu} \right]^{(m_i+\nu_i/2)} \exp\left(-\frac{\overline{\Gamma}_o}{\overline{\Gamma}} \frac{1-\mu}{1+\mu}\right) d\mu . \tag{13}$$

In these expressions, $\overline{\Gamma}_o$ is the sum of all non-fluctuating widths, e.g., Γ_γ, and n is the number of fluctuating widths. Here m_i=0, 1 or 2 depending on whether reaction width Γ_i appears as a factor zero, once or twice, respectively in the numerator of the left hand side of Eq. 12. For example: assuming Γ_x=0 for elastic scattering m_n=2, n=1; for neutron capture assuming Γ_γ constant for all resonances m_n=1, m_γ=0, n=1, for fission m_n=1, m_f=1, n=2.

Equation 13 is evaluated in the code by means of Gaussian Integration utilizing 20 points over the range $-1 \le \mu \le +1$ taken at the zeros of the Legendre Polynomials of order 20. The abscissas and weights used are given in Table M.1 of Appendix M. It is also shown there that calculational errors using this scheme are completely negligible.

b) <u>Method of MC^2</u>

It is assumed that the competitive reaction width is zero and that Γ_γ^s is constant. Then Eq. 6 gives the cross section for non-fissile materials. For fissile isotopes, an integration over the chi-squared distribution, $S_k(y)$, for the fission widths must also be included in Eq. 6, where $y = \Gamma_f(E)/\overline{\Gamma_f(E^*)}$. The mean fission width is tabulated as a function of energy on the data tape.

The integration over the chi-squared distributions is performed as it is in MC^2, employing 10-point integration for one or two degrees of freedom in the neutron width distribution, and five-point integration for one to five degrees of freedom in the fission width distribution. Values of z_i are determined such that:

$$\int_{z_i}^{z_{i+1}} S_j(w)\,dw = \frac{1}{N}$$

where N = 10 and 5 for the neutron and fission width distributions, respectively, and $z_0 = 0$, $z_n = \infty$. Within each interval (z_i, z_{i+1}), average values of w are computed from the relation,

$$w_{i+1} = N \int_{z_i}^{z_{i+1}} w' S_j(w')\,dw'$$

The program then assumes that

$$\int_0^{\infty} f(w') S_j(w')\,dw' = \frac{1}{N} \sum_{i=1}^{N} f(\chi_i)$$

Tables 2.2 and 2.3 taken from Appendix A of Reference 6 list the values of w_i used in SAM-X.

TABLE 2.2 - VALUES OF w_i USED FOR INTEGRATION OF NEUTRON-WIDTH DISTRIBUTIONS WITH ONE OR TWO DEGREES OF FREEDOM

	Degrees of Freedom, n	
Index, i	1	2
1	0.0052543	0.051755
2	0.037174	0.163089
3	0.103133	0.288398
4	0.20785	0.43172
5	0.359875	0.599144
6	0.57432	0.800477
7	0.879486	1.05263
8	1.33502	1.39297
9	2.10558	1.91582
10	4.3923	3.304

TABLE 2.3 - VALUES OF w_i USED FOR INTEGRATION OF FISSION-WIDTH DISTRIBUTIONS

	Degrees of Freedom, n			
Index, i	1	2	3	4
1	0.0212093	0.1074	0.189269	0.254966
2	0.155477	0.36007	0.476304	0.549072
3	0.467072	0.699863	0.793185	0.842565
4	1.1071	1.22312	1.23576	1.23075
5	3.24914	2.60955	2.30575	2.12265

2.3.2 Treatment of Smooth Cross Section Data

File 3 of the ENDF data tape consists of more than one section, each containing smooth cross section data for a particular type of reaction. A list of numbers MT and associated reaction types utilized by SAM-X is given in Table 2.4.

TABLE 2.4 - LIST OF NUMBERS MT AND ASSOCIATED REACTION TYPES UTILIZED BY SAM-X

MT	Reaction Type
1	Total
2	Elastic
3	Nonelastic
4	Total inelastic (sum of MT=51,52,...,91).
5-15	Not used
16	(n,2n)
17	(n,3n)
18	Fission=(n,f)+(n,n'f)+...,
19	(n,f)
20	(n,n'f)
21	(n,2nf)
22	(n,n')α
23	(n,n')3α
24	(n,2n)α
25	(n,3n)α
26	Not used
27	Absorption (fission + capture)
28	(n,n')p
29	Scattering (elastic and inelastic)
30-50	Not used
51-90	(n,n') (inelastic levels)
91	(n,n') (inelastic continuum)
92-100	Not used
101	Parasitic absorption (sum of MT=102, 103,...,109)
102	(n,γ)
103	(n,p)
104	(n,d)
105	(n,t)
106	(n,He^3)
107	(n,α)
108	(n,2α)
109	(n,3α)

Since detailed flow (in program OVER13) is described later, only a number of assumptions made in the routine are discussed here.

1. Absorption, scatter, and inelastic cross-section tables as required by the SAM-F program are generated. A fourth quantity calculated, dependent upon input control word IMULT, is either the multiplicity or the fission cross section.* The multiplicity, m(E), at energy E is defined as

$$m(E) = \frac{\sum_r N_r \sigma_r(E)}{\sum_r \sigma_r(E)}$$

where N_r is the number of neutrons emitted in reaction type r, and the sum is taken over "inelastic" reactions. As is indicated below, many reaction types for which data are given explicitly on the ENDF tape are combined to generate the absorption and inelastic cross sections for use in SAM-F.

2. The program assumes that all components of composite cross sections are given in File 3 if the composite, e.g., nonelastic, inelastic, absorption, parasitic capture, total scatter, is given. Only the composite inelastic cross section data (MT=4) are utilized and must be given if the components are given.

* Only the multiplicity option is relevant to SAM-F (see Input Description, Section 2.5).

3. The following reaction types are treated as components of the absorption cross section: (n,γ), (n,p), (n,d), (n,t), (n,He^3), (n,α), (n,2α), (n,3α).

   In addition, the fission cross section is included in the absorption cross section when the multiplicity for inelastic scattering is calculated for use in SAM-F.

4. The following reaction types are treated as components of the inelastic cross section: (n,n'), (n,2n), (n,3n), (n,n')α, (n,n')3α, (n,2n)α, (n,3n)α, (n,n')p.

5. If resonance cross sections have been generated in interval (E_1,E_2) by program OVER12, the output energy mesh outside of the interval is determined by use of the File 3 input tables for reaction types MTABLO and MTABUP, entered as card input. Reaction types MTABLO and MTABUP determine the energy mesh below and above the resonance range (E_1,E_2), respectively. If no resonance cross sections have been generated, the two reaction type numbers inputted determine the output mesh below and above energy EN1, entered as card input. Points are added to the output energy table to assure that cross sections calculated at intermediate points by use of both linear interpolation

and the interpolation scheme designated by ENDF agree within input criterion EPSI.

2.3.3 Treatment of Secondary Angular Distributions

Secondary angular distributions, expressed as normalized probability distributions, are given in Files 4 and 14 of the ENDF tape. Program OVER15 (see Fig. 2.2), and its supporting subroutines process elastic angular distributions (MT=2) and discrete inelastic angular distributions (MT=51,...,90). Similar coding exists in PEND for File 14 (Photon Angular Distributions). These distributions may be presented either in tabulated form, normalized such that

$$\int_{-1}^{1} p(\mu,E)\,d\mu = 1,$$

or as Legendre coefficients, $f_\ell(E)$, defined by

$$\frac{d\sigma(\mu,E)}{d\Omega} = \frac{\sigma_S(E)}{2\pi} \sum_{\ell=0}^{NL} \frac{2\ell+1}{2} f_\ell(E)\,P_\ell(\mu) \equiv \frac{\sigma_S(E)}{2\pi}\,p(\mu,E)$$

where the angular variable μ may refer to either the laboratory or center-of-mass coordinate system ($\mu=\cos\theta$, where θ is the angle of scattering).

The given angular distributions are represented on the EDT by a table of percentiles (x-table)* in the center-of-mass coordinate system, where

$$x \equiv \frac{1-\mu}{2} \tag{14a}$$

If N x-values are given, N+1 equally probable angular bins are defined (with $x_o=0$ and $x_{N+1}=1$ as implied bin boundaries). The distribution is assumed to be uniform in each bin.

---

* Also referred to as "chi table."

The distribution $p(\mu)$ (assuming conversion to center-of-mass if originally given in laboratory system) is, therefore, represented by $q(x)$, where

$$q(x) = \frac{1}{(N+1)(x_{n+1}-x_n)}; \quad x_n \le x \le x_{n+1}; \; n=0,1,\ldots,N \qquad (14b)$$

The x-values are determined from the solution of:

$$\frac{n}{N+1} = \int_{1-2x_n}^{1} p(\mu)d\mu, \; n=1,2,\ldots,N \qquad (15)$$

In program FILE4 (as well as in PEND), N is determined to be the smallest integer such that four criteria are satisfied:

(1) N is a non-decreasing function of energy;

(2) the ℓ-th moment of the angular distribution (as represented) does not deviate from the ℓ-th moment of the given distribution by more than ε_ℓ for $\ell=1,L$ (L and ε_ℓ, $\ell=1$, L are read as card input);

(3) the fractional deviation of the angular distribution (as represented) from the given distribution does not exceed α ($\alpha>0$ read in as card input);

(4) N does not exceed LADHOC (a number read as card input);

The calculation of the x-values by equation (15) begins by setting N=0 for the lowest energy angular distribution. Criteria (2) and (3) are tested and if either test fails, N is incremented by 1, and a new set of x-values is computed. When the criteria

are satisfied, the angular distribution at the next higher energy is processed, with N initialized to its value at the preceding energy.

The x-calculation and the testing of criterion (3) proceed concurrently in subroutine CALCHI. As soon as x_{n+1} is computed, the given distribution $p(\mu)$ is examined in the interval $(1-2x_{n+1} < \mu \leq 1-2x_n)$ for the maximum entry p_m; the value α is compared to the test value

$$1 - \frac{1}{2(N+1)(x_{n+1}-x_n)p_m}; \quad p_m \geq 0.5 \tag{16a}$$

or, for $p_m<0.5$ (= average value of p) the test is relaxed to a comparison with the value

$$2p_m - \frac{1}{(N+1)(x_{n+1}-x_n)}; \quad p_m<0.5 \tag{16b}$$

If the test value exceeds α, N is incremented by 1 and the calculations of the x_n-values are restarted with n=1.

Criterion (2) can be performed only after all N x-values have been calculated. The ℓ-th moment, M_ℓ, of the distribution (as represented) is given by

$$M_\ell = \sum_{n=0}^{N} \frac{1}{2(N+1)(x_{n+1}-x_n)} \int_{1-2x_{n+1}}^{1-2x_n} P_\ell(\mu)d\mu \tag{17a}$$

The M_ℓ are computed in subroutine MOMNTX using the relations

$$\int_{x_1}^{x_2} P_\ell(x)\,dx = \frac{1}{2\ell+1}\left[P_{\ell+1}(x_2) - P_{\ell+1}(x_1) - P_{\ell-1}(x_2) + P_{\ell-1}(x_1)\right] \tag{17b}$$

$$P_0(x) = 1 \tag{17c}$$

$$P_1(x) = x \tag{17d}$$

$$P_\ell(x) = \frac{1}{\ell}\left[(2\ell-1)xP_{\ell-1}(x) - (\ell-1)P_{\ell-2}(x)\right] \tag{17e}$$

The ℓ-th moment of the given distribution, f_ℓ, is known if Legendre coefficients are given, or computed in subroutine MOMENT if the given distribution is tabulated. Hence, as soon as M_ℓ is computed, the test $|M_\ell - f_\ell| : \epsilon_\ell$ is performed in MOMNTX. If $|M_\ell - f_\ell| > \epsilon_\ell$, N is incremented by 1 and the calculation of a new x-table is initiated. Otherwise, ℓ is incremented by 1 and the next M_ℓ is tested. Criterion (2) is satisfied when $\ell > L$.

If at any stage of the x-calculation N=LADHOC, testing of criteria (2) and (3) is bypassed and N x-values are computed for the remainder of the angular distributions.

2.3.4 Secondary Energy Distributions

Secondary energy distributions, given in File 5 of ENDF, are expressed as normalized probability distributions, $p(E \to E')$ where

$$\int_0^\infty dE'\ p(E \to E') = 1 \tag{18}$$

Furthermore, the distribution is expressed as

$$p(E \to E') = \sum_k p_k(E) f_k(E \to E') \quad (19)$$

so that different distributions in different energy ranges can be accommodated. As seen from substitution of Eq. 19 into Eq. 18, the $f_k(E \to E')$ are normalized in the same way as the $p(E \to E')$. The $f_k(E \to E')$ may be specified in several ways, designated by the index LF.

Distributions for inelastic scattering reaction types only are required to generate the necessary data for the SAM-F EDT. Although six different representations of secondary energy distribution are currently defined, the cases that SAM-X will handle are listed in Table 2.5. These are the cases which are relevant to the SAM-F EDT.

TABLE 2.5 - SECONDARY ENERGY DISTRIBUTION REPRESENTATIONS HANDLED BY SAM-X

Control Word, LF	Representation of Distribution
1	General tabulated function.
3	Discrete level excitation.
4	General evaporation spectrum, $g(E'/\theta)$, θ = nuclear temperature is constant.
5	Same as 4, but $\theta = \theta(E)$.
7	Simple fission spectrum.
8	Maxwellian, $g(E') = E'/\theta^2 e^{-E'/\theta}$, with θ = constant.
9	Same as 8, but $\theta = \theta(E)$.

The SAM-F EDT requires that the energy distribution of inelastically scattered neutrons be specified at each output energy above the threshold. If a discrete component exists, two tables are established:

1. Table of excitation energies, ELEV(I), where I varies from 1 to LPLEV, the number of discrete levels; and

2. Table of cumulative excitation cross section designated as PLEV(I), where I varies from 1 to LPLEV, and PLEV(I) is the sum of the excitation cross sections of the 1^{st} through the I^{th} levels.

If a continuous spectrum component exists, the table of equiprobable energies after (inelastic) scattering is established. At each output energy E, the entries ENN(I) are defined to be the solutions of the equation:

$$\int_0^{ENN(I)} q_c(E \to E')dE' = \frac{I-1}{N-1} \int_0^E q_c(E \to E')dE', \quad I=1,2,\dots,N \tag{20}$$

where $q_c(E \to E')$ is the continuous component of the distribution of neutrons scattered inelastically from energy E to E', and N, equal to input quantity LENN, is the number of entries in the table at E. Although SAM-X permits only one reaction type with a discrete spectrum component, no limit is set on the number of reaction types contributing continuous components. Therefore, if use is made of Eq. 19, $q_c(E \to E')$ may be expressed as:

$$q_c(E\rightarrow E') = \frac{\sum_k \sigma_k^{in}(E)n_k \sum_\ell p_\ell(E)f_\ell(E\rightarrow E')}{\sum_k \sigma_k^{in}(E)n_k \sum_\ell p_\ell(E)} \qquad (21)$$

where $\sigma_k^{in}(E)$ is the inelastic cross section at E, and n_k is the number of neutrons emitted in reaction type k. At each output energy E, $q_c(E\rightarrow E')$ is computed at 201 equally spaced energy points E' from 0 to E. The integral on the right-hand side of Eq. 20 is evaluated at these points, stored in a table, and the values of ENN(I) are computed by means of linear interpolation in the table.

2.3.5 Treatment of Photon Production Data

The PEND processor of SAM-X (details of code organization are given in Section 2.4) produces a gamma production data tape (GPDT) from the photon production files of an ENDF tape. The GPDT output by PEND serves as input to both SAM-F and SAM-A (see Figure 1.1) for forward and adjoint secondary gamma ray transport solutions, respectively. This GPDT may be saved for future SAM-F and SAM-A runs.

The organization of a GPDT is presented in Appendix D. The current version of PEND is now equipped to process File 14 (Photon Angular Distributions), as discussed in Section 2.3.3.

From the diversity of information on the ENDF files, the essential data which must be retrieved are the photon yields tabulated for a two-dimensional grid of energies corresponding to the incoming neutron energy and the outgoing photon energy. For a given photon of energy E_γ, the yield $Y_\gamma(E)$ is defined as

$$Y_\gamma(E) = \sigma_\gamma(E)/\sigma_{ne}(E)$$

where $\sigma_\gamma(E)$ ' the gamma production cross section for the reaction which yields the photon of energy E_γ, and $\sigma_{ne}(E)$ is the total non-elastic cross section at neutron energy E.

Tabulations of $\sigma_{ne}(E)$ are readily retrievable from an existing neutron element data tape (NEDT). This presupposes that the neutron data has already been produced by the NUTRON processor of SAM-X. Hence, the main task of the PEND processor is to produce tabulations of $\sigma_\gamma(E)$ for each E_γ. The E_γ set will include whatever discrete photons are specified, plus a set of "photons" discretized by the integration of the continuous spectra.

2.3.5.1 Multiplicities

In the ENDF File 12 photon multiplicities may be tabulated directly (option LO=1), or must be extracted from transition probability arrays (option LO=2). In either case, the yields are not the $Y_\gamma(E)$ defined above, but are the yields, given that a specific reaction type (i.e., fission, radiative capture, etc.) has occurred. This means that the corresponding neutron cross sections must be known. These partials are not retained on the NEDT; they must be computed from the information in the ENDF File 2 and/or File 3.

The current version of PEND is capable of processing the File 12 photon multiplicities if the interdependence with neutron cross section data only involves File 3 (Smooth Cross Sections). At present, there is no coding for option LO=2. The available routines will extract photon multiplicities which are directly tabulated (option LO=1) and will combine these with File 3 cross sections to produce photon production cross sections analogous to the tabulations produced from File 13 data.

2.3.5.2 Photon Production Cross Sections

The photon production cross sections given in ENDF File 13 are tabulated by PEND on the basic energy mesh established for the NEDT. Due to the potentially large number of neutron energies, however, only the "non-zero" (using a nanobarn cutoff) values between two energy bounds will be saved. The procedure is described in corresponding subsections of Section 2.4.

2.3.5.3 Anisotropy of Photon Production

Should data exist in File 14 giving anisotropy of photon production, PEND will process these data and organize them into the format recognized by SAM-F and SAM-A.

2.3.5.4 Continuous Photon Energy Spectra

A discretized set of photons is computed by PEND from the continuous spectra given in ENDF File 15. A default set of "photon energies" and corresponding energy intervals for integration is specified internally, with provision for user override. The contributions from all given spectra (corresponding to different reaction types) are superimposed. The procedure is described in corresponding subsections of Section 2.4.

2.3.5.5 Data Reduction

The data reduction of a GPDT is accomplished by the WEED processor in two modes, termed "weeding" and "binning." In the weeding mode, neutron energy mesh points and their corresponding yields are eliminated in accordance with a linear interpolation criterion between neighboring mesh points. The second mode involves reduction of data through the binning (or superposition) of photons in accordance with a relative energy interval criterion and an overall GPDT length limit. The details of this procedure are given in the corresponding subsection of Section 2.4.

2.3.6 Treatment of Photon Cross Section Data

GAMMA, the fourth primary overlay of SAM-X, processes the ENDF photon cross section data into the format recognized by SAM-F and SAM-A.

In general, the format of the gamma element data tape (GEDT) resembles the format of the neutron element data tape (NEDT) but is considerably smaller in size and in the number of options necessary to present the data.

The organization of the GEDT is given in Appendix B.

2.3.7 EDT Conversion

The ENDF processing routines, NUTRON, PEND, WEED and GAMMA, produce an EDT written in binary blocks of 510 words - which is how SAM-F and SAM-A read the EDT. This makes the original EDT machine dependent.

To nullify the machine dependence of the EDT, program BCDEAN may be used. This program serves as a two way EDT converter, i.e., binary-to-BCD and vice versa.

There are two basic modes, then, for using BCDEAN:

1) In the binary-to-BCD mode, the conversion is performed for one element sequentially as the other overlays of SAM-X process an NEDT, GPDT (by PEND or WEED) and GEDT, or any partial sequence. The output EDT is in sequenced card image format and includes a provision for appending descriptive text.

2) In the reverse mode, BCD-to-binary, BCDEAN operates essentially as a stand-alone code, and can, therefore process any number of EDT's in a single execution.

The structure of the BCD EDT produced by BCDEAN is described in Appendix N.

2.4 SAM-X - Information Flow

The SAM-X code comprises a main overlay (SAM-X), five primary overlays (NUTRON, PEND, WEED, GAMMA, and BCDEAN), and seven secondary overlays subordinate to primary overlay NUTRON. The gross structure of the SAM-X code is shown in Figure 2.2.

Except for the main and third primary overlay, all the overlay directives specify a first word address (relative to the start of blank common) for loading. In this manner, the dimension of blank common is varied from a minimum of 5022 (decimal) required by GAMMA to a maximum value, currently specified as 30.6K (decimal) in SAM-X, all of which is also available in WEED.* The 30.6K (decimal) dimension corresponds to 60 blocks of 510 words, the I/O unit of an EDT. Although 50 I/O units would have sufficed in most situations, the additional 10 I/O units made the total memory requirement for loading WEED approximately equal to the memory required to load NUTRON with OVER15 (the longest branch of the first primary overlay). Similarly, the intermediate address of 61634 (octal) corresponds to a blank common dimension of 25.5K (decimal), or 50 I/O units, in PEND, whose memory requirement (strictly for coding) is intermediate between the requirements for (NUTRON + OVER15) and for WEED. Finally, the loading address specified for all the secondary overlays was determined from the memory required to load NUTRON alone; this address insures that the secondary overlays, subordinate to NUTRON, are loaded contiguous with the end of NUTRON.*

---

* The absence of an explicit loading address in a secondary overlay directive implies that the secondary overlay is loaded at the end of its primary, or blank common, whichever address is higher.

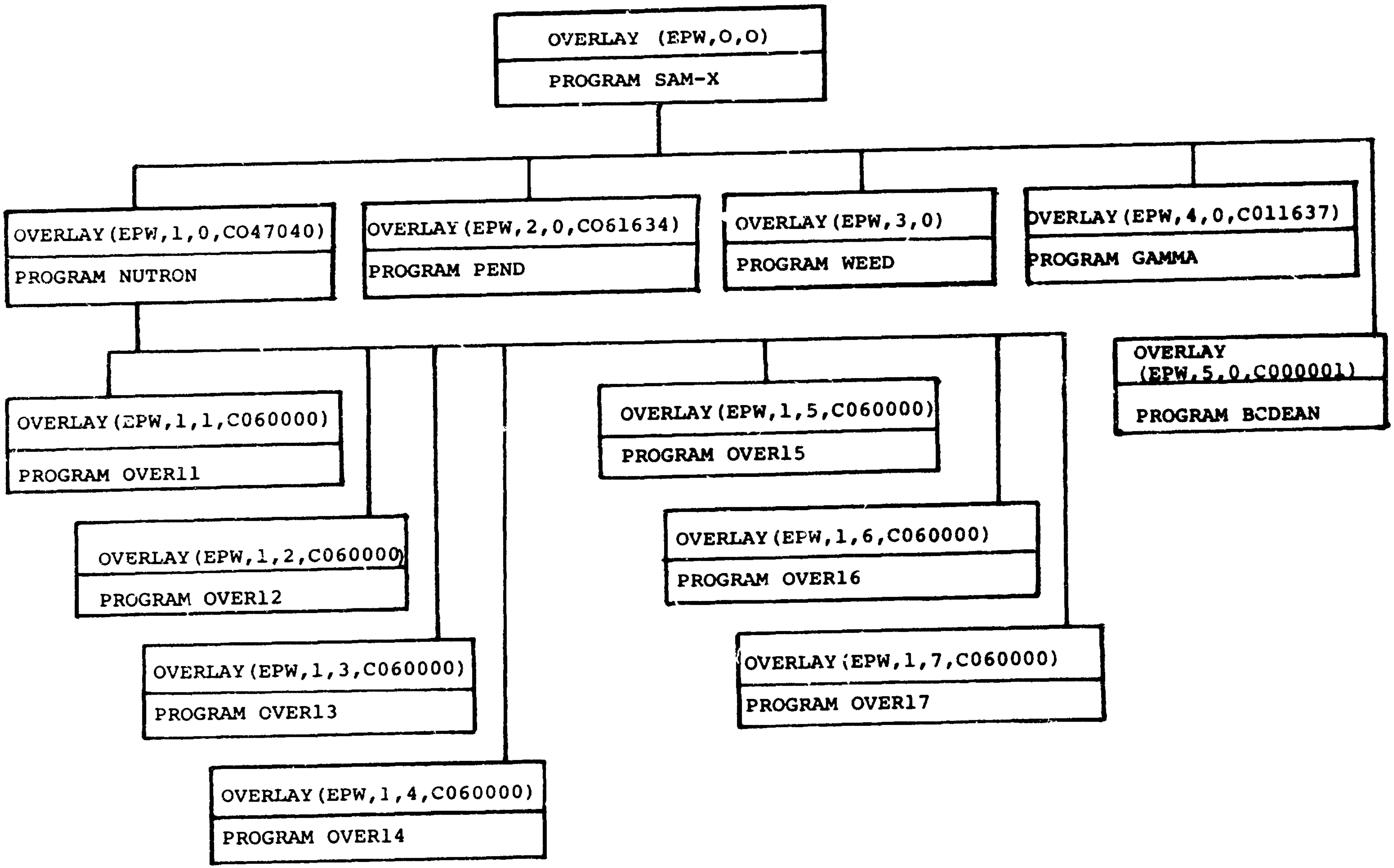

Figure 2.2 Gross Structure of SAM-X

In the subsections that follow, each overlay will be given a detailed discussion, which in conjunction with the comment cards of the FORTRAN listing, should aid a programmer in making changes to the present version of the code.

The main overlay program, SAM-X, controls the call to the five processors via card input. The user can specify a complete sequential execution (NUTRON, PEND, WEED, GAMMA, and BCDEAN) a partial sequence, for example, (PEND, WEED), or an individual execution of any one processor. The partial sequence (. WEED) or an individual execution of PEND presupposes the availability of the corresponding NEDT from a previous execution of NUTRON. The individual execution of WEED presupposes the availability of a GPDT from a previous execution of PEND (or WEED). An execution of BCDEAN presupposes a prior execution of one of the first four processors.

Another function of the main program is to define all I/O devices and to specify blank common dimensions for the five primary processors, transmitted by labeled common/PEW/ and/or implied by the loading directives, for NUTRON as LENTAB words (see Section 2.8) and 5022 for GAMMA. BCDEAN does not utilize blank common.

The main overlay includes one subroutine, DSPLAY. This routine, utilized by PEND, WEED, and GAMMA, displays a singly dimensioned array, ten entries per line (with a cumulative count written in the 11th column). The portion of the array to be displayed is specified by two arguments in the call, viz.

CALL DSPLAY(name(i), ℓ)

where name is the array name, i and ℓ are first and total number of entries to be displayed, respectively. The format for each entry is either E11.4 or I11, the appropriate format being determined internally.

2.4.1 NUTRON (OVER10)*

NUTRON, controlling the call to various secondary overlays, is the main program of the neutron processor, in which most card input is read for processing the neutron ENDF files. An additional function, performed prior to the call to OVER13 if resonance cross sections for individual isotopes of a material have been generated, is the combining of such cross sections into one composite table which is written on logical tape NTAPW. The following routines, loaded with NUTRON, are used by NUTRON and/or one or more of its secondary overlay programs.

PRHED

This subroutine is called to restore and number the output pages, and to print the input heading at the top of each page. It also calls TIME and prints the elapsed time in seconds from start of execution.

COMBIN

This routine is called to combine partial cross sections generated on different energy meshes into a composite cross section table. These data may have been generated for different reaction types of a given isotope or for different isotopes of a given material. The cross sections appear on logical tapes NTAPR, NTAPT, and NTAPW, where NTAPR contains the last composite cross section generated, NTAPT contains the cross sections to be combined with those on NTAPR, and NTAPW contains the combined data. Use of these tapes was necessitated by lack of memory storage capacity.

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* See second footnote, p. 15.

MERGET

This routine, called by COMBIN, performs the merging of the cross section tables as described above, adding together, when necessary, the various contributions to the cross sections calculated. (No addition occurs when the subroutine is employed in establishing the output energy table.) In this calculation of cross sections from data generated at points intermediate to the output energies, linear interpolation is used, since cross sections generated are required to be linear within an input criterion. Merging continues until all input data records on tapes NTAPR and NTAPT, together with any required cross sections stored in memory, have been processed and combined.

RITRC

This subroutine, called by a number of routines including MERGET, writes two records on logical tape NTAPW; the first record gives the length of the record to follow which contains tables of energies and cross sections extending over a limited range of energies. The routine, written to overcome core storage limitations, is used to write cross sections on tape in records of NUMWD words or less during the generation of the cross section table extending over the entire energy range of interest. NUMWD is entered as card input to SAM-X.

REDRC1

This routine reads two records from logical tape NTAPR; the first record gives the number of words in the second record which contains the energy and cross section tables to be merged with an existing table.

REDRC2

This routine is the same as REDRC1, except that logical tape NTAPT is read.

SKIP

This subroutine is used to skip over a section, file, or material on the ENDF data tape when its argument N is entered as 3, 2, or 1, respectively.

REDLIST

This subroutine is called to read a list record, as described in Reference 1, from the ENDF data tape. Such a record is a string of floating point numbers such as the energies at which fission widths are tabulated as requested in OVER12, or the transformation matrix read in OVER15.

NTERPL

This routine is called to perform an interpolation in a tabulated function, $\sigma(E)$. One of five permissible interpolation schemes, i.e., constant, σ linear in E, σ linear in ln E, ln σ linear in E, ln σ linear in ln E, is selected when argument IN is entered as 1, 2, 3, 4, or 5, respectively. E_1 and E_2, values of the independent variable which bracket the value of E at which the result is desired, are transmitted to the routine together with corresponding values SIG1 and SIG2 of the dependent variable. SIG, the desired result at E, is transmitted to the calling program by means of the common block, /INTERPL/.

TIME

This routine, called by PRHED, computes elapsed time in seconds by interrogating the machine clock routine.

2.4.1.1 OVER11

After the card input describing the materials whose cross section and distribution tables are to be generated has been read, OVER11 is called. The program locates a desired material on the ENDF data tape by comparison of material identifier, ZA, on tape with input identified ZAP(I). Then variables are initialized, and Hollerith information describing the sources of data and their evaluation (including the dictionary) is read and printed. The only other piece of File 1 data employed, not required by SAM-F is that describing ν, the number of neutrons produced per fission. The code accepts the data, expressed as a polynomial in incident neutron energy (in Mev), retains terms up to second order, and stores the coefficients. If the data are tabulated, a least-squares fit must be performed by subroutine LSQFT before the coefficients can be stored.

REDTAB1

This subroutine is called in a number of programs - OVER11, OVER13, OVER16-to read a TAB1 record from the ENDF data tape which, as described in Reference 1, is a tabulation of y(x) vs x given together with an appropriate interpolation scheme. In the call from OVER11, the table of ν(E) vs E is read.

LSQFT

This routine computes the coefficients of a polynomial of second degree for y(x), given a tabulation of y(x) vs x. A standard least-squares fit is performed by solving the three simultaneous

equations generated. In the case of the call to LSQFT made by OVER11, the coefficients of $\nu(E)$ are calculated when $\nu(E)$ is tabulated on the ENDF data tape.

2.4.1.2 OVER12

The reading of File 2 data is initiated by program OVER12. If resonances are given for individual isotopes, cross sections are generated for each isotope, usually on different energy meshes, and then written on tape to be combined later after all resonance data have been processed. If data exist in the energy range of interest, the program, either by itself or through subroutine calls, reads resonance parameters before the call to RESON for the generation of cross sections in the two ranges. Resolved resonance parameters are read by Subroutine REDPAR. Unresolved resonance parameters which are energy-independent are read by RDPARU. Energy-dependent unresolved parameters are read by the program itself. For fissile elements, the fission widths may be energy-dependent with all other resonance parameters energy-independent. A call is made to REDLIST to read the energy tabulation points of the fission widths. This is followed by the call to RDPARU. Before control is returned to the main program, SAM-X, upon exit from OVER12, the bounds of the resonance region are stored for later use in OVER13 where the cross sections are generated for the entire energy range of interest.

REDPAR

This subroutine is called to read and print resolved resonance parameters $E_r, J_r, \Gamma_r, \Gamma_{\gamma r}, \Gamma_{fr}$ for all resonances, as defined in Section 2.3.1.1.

RDPARU

This routine is called to read and print energy-independent unresolved resonance parameters, $D_r, J_r, \mu_{nr}, \Gamma_n^0$, and Γ_γ where D is the mean

level spacing, μ_{nr} the number of degrees of freedom used in the neutron width distribution, and Γ_n^0 the average reduced neutron width. If the data exist, the number of degrees of freedom used and the distribution of average fission widths at energies already read in OVER12 are read and printed.

RESON

This routine simply calls subroutine RES and UNRES, respectively, to generate the resolved and unresolved resonance cross sections for an individual isotope, and then writes the entire set on logical tape 9.

RES

This subroutine performs the calculation of cross sections in the resolved resonance range. The code, while establishing the output energy mesh as described in Section 2.3 calculates cross-section contributions of individual resonances by means of the single-level Breit-Wigner formula and sums over the resonances in a given sequence. Only those resonances whose peak energies lie within WIDTHS total widths of the energy at which the cross section is computed are included in the sum.

If requested, the routine calculates a variable convergence criterion EPS for material M in the resolved range. At a given energy E

$$\mathrm{EPS} = \mathrm{EPSI(M)} + \ln\left(\frac{\mathrm{E}}{\mathrm{EA}}\right)\left[\frac{\mathrm{EPSJ(M)} - \mathrm{EPSI(M)}}{\ln\ (\mathrm{EP/EA})}\right] \qquad (22)$$

i.e., a logarithmic variation of EPS is assumed from EPSI(M) at EA, the lower bound of the resolved resonance range, to EPSJ(M) at EB, the upper bound.

During the calculation, subroutine FACTRS is called to compute penetration factors, shift factors, and phase shifts, subroutine W to Doppler-broaden the cross sections, and TEGRAT to perform the Trapezoidal Rule integration of the cross section curve in the establishment of the output mesh. Cross sections calculated at the upper end of each energy interval during the establishment of the mesh are saved if the convergence criterion is not met (NTEST=1); then the interval is subdivided further as described in Section 2.3.1.1. These quantities are picked up again when the convergence criterion has been met (NTEST=2), and the routine moves on to treat the next higher energy interval.

Partial cross sections are stored in the variable TAB array, and dumped on tape NTAPW by call to RITRC when either NUMWD words of energies and cross sections have been stored or the generation of isotopic cross sections has been completed. When all the cross sections for the various ℓ states of the individual isotope have been generated in the resolved range, subroutine COMBIN is called to merge the partial cross sections into a composite table. A note should be made here about the use of the TAB array. In order to overcome the lack of memory storage capacity, individual allocations are obviated by storing input arrays, energy, and generated cross section tables in the LENTAB word TAB array,* and by the use of indices to keep track of the origins of the various types of data.

* See Section 2.8.

FACTRS

This routine is called by RES to calculate the penetration factors (PENFL), shift factors (SHIFL), and phase shifts (PHIL) at each desired energy and ℓ-state. Equations used, taken from Reference 1, are given in Table 2.1. To reduce running time, phase shifts are calculated only when required in the computation of the cross section.

W

W is a routine written by O'Shea and Thacher[5] for the rapid computation of the resonance line shape functions ψ and χ as the real and imaginary parts of the complex probability integral.

TEGRAT

This routine performs the Trapezoidal Rule integration of the absorption or total cross section, if INTEST is entered as 0 or 1, respectively. For a given energy interval, cross sections computed at the end points and at the midpoint are transmitted to the routine by means of common block /TEGDEP/. The integral over the whole interval, GR(1), is compared to the sum of the two integrals taken over each of the half-intervals, GR(2) + GR(3). If these quantities agree within input convergence criterion EPSI, i.e., $|1-r| < \text{EPSI}$, where r is the ratio [GR(2)+GR(3)] /GR(1), then the energy, E_u, and cross section, σ_u, at the upper end of the interval are stored in the output table (NTEST=2); control is then returned to the calling program, RES. If the two terms do not agree within the convergence criterion, (NTEST=1), E_u and σ_u are stored in memory for later use

in establishing the output mesh; then the lower half-interval is halved, replacing the whole interval in the procedure outlined above. The precedure is followed until the two terms agree within EPSI. Any energies and cross sections stored previously ($J \geq 2$) are then retrieved, in turn, as the next higher subinterval is treated. (Note: The maximum number of energies or cross sections which may be stored is 30, at which point the upper bound of the last subinterval stored is placed in the output table.)

UNRES

This routine, either by itself or through subroutine calls, performs the calculation of cross sections in the unresolved range, as discussed in detail in Section 2.3.1.2. Correct indexing of resonance parameters in the memory locations of the TAB array is maintained throughout the routine for the three allowed ENDF formats, i.e., energy-independent parameters for non-fissile elements, energy-independent parameters for fissile elements, and energy-dependent parameters for both fissile and non-fissile elements. After retrieval of the resonance parameters from memory, the cross sections are calculated. For the default option, JUNIN=2, this is accomplished by a call to subroutine GAUSIN. For the MC^2 option, JUNIN=1, the calculation is done within the routine itself. The cross sections are written on logical tape NTAPN after they have been generated; then a call to subroutine COMBIN establishes a composite table of resonance cross sections by merging the unresolved data with already existing resolved data.

GAUSIN

This routine is called by UNRES for the option JUNIN=2. It computes the distribution average of $\left\langle \Gamma_n^3 \Gamma_i^s / \Gamma^s \right\rangle$ for elastic scattering, neutron capture and the fission reaction (if required) as specified by Eq. 12 and 13. The Gaussian quadrature technique is utilized as discussed in Section 2.3.1.2.

TBSEEK

This routine is called by UNRES when resonance parameters are given in the energy-dependent ENDF format. This binary search routine is utilized to find the indices within the TAB array that specify the energy points enclosing an E*, a discrete energy point at which the cross sections are tabulated. After return to UNRES, a call to subroutine NTERPL calculates the cross sections at E* using the interpolation scheme specified in the ENDF data.

BLOCKDATA

The BLOCKDATA statement is used to specify the 20 abscissas and weights utilized in the Gaussian quadrature calculation in GAUSIN. These are stored in common block LGN.

2.4.1.3 OVER13

The OVER13 program reads and processes the information given in File 3 of the ENDF data tape. The code reads the data tape, logical unit 10, while looking for reaction type MT equal to MTABLO, entered as input for the material being treated. If reaction types are encountered before MTABLO is found, the data for these reactions are copies onto logical unit 9. When MT=MTABLO is found, the table is read by subroutine REDTAB1, and employed by ADE in establishing the output energy mesh below the lower bound of the resonance range, defined in OVER12. If no resonance information is given on the data

tape, the energy breakpoint, below which the output mesh is established by the table for reaction type MTABLO, is set equal to input quantity EN1. If reaction types MT=51,...,91 are encountered, the data for these reactions are copied onto logical unit 17 for later processing in the OVER16 program. Consequently, neither MTABLO nor MTABUP can be set to these MT values.

An index M is set up to permit the storing of cross sections in their proper place in the output table; each energy is followed by the corresponding absorption, scatter, inelastic, and fission (multiplicity) cross sections for which M is set equal to 1, 2, 3, 4, respectively. After the energy mesh below the "resonance" range has been established, existing (resonance) cross sections are read from logical tape NTAPR in records of NUMWD words or less, added to the smooth cross sections for reaction type MTABLO, and written on logical tape NTAPW. If no resonance data have been generated (IRIT4=0), the table for reaction type MTABLO determines the mesh on which the cross sections are written on NTAPW to be combined later with cross sections of other reaction types. Then tape NTAPW becomes the tape from which existing cross sections will be read (designated NTAPR) during the processing of data for the next reaction type considered.

The code continues to read logical unit 10, searching for reaction type MTABUP, entered as input for the material being treated. If desired reaction types are encountered before MTABUP is found, these data are copied onto logical unit 9. The table

for MTABUP, when found, is read by REDTAB1 and employed by ADX in establishing the output mesh above the upper bound of the defined resonance range, or above EN1 if no resonance data exist. Cross sections are read from tape NTAPR and added to the smooth cross sections for reaction type MTABUP in the desired mesh in subroutine ADX. If the data for MTABUP are not found on logical unit 10, the code searches logical unit 9 for the table and establishes the output mesh. OVER13 then rewinds tape 9 and processes the File 3 data for the other reaction types on the tape, skipping over MTABUP when encountered. After the table for a reaction type treated as inelastic has been read, the nonzero File 3 data are copied onto logical tape 15 for later use in OVER16 during the processing of the energy distribution data (File 5).

It is to be noted here that a number of reaction types are bypassed, and an appropriate comment printed. As stated in Section 2.3.2, composite cross sections such as total, nonelastic, absorption, and total scatter are not utilized since it is assumed that data for all components of these cross sections are given.

Some coding from a predecessor code still exists for the treatment of temperature-dependent smooth cross sections. Although this coding is no longer valid, it has been retained to serve as a guide to required programming changes when this option is made operational.

ADVAMT

This routine is called by OVER13 to read the ENDF data tape, logical unit 10, and copy the File 3 data for individual reaction types onto logical unit 9 or 17 as the data tape is searched for reaction type MTABLO or MTABUP.

TESTMT

This routine is called when multiplicity is being calculated, and sets up the number of neutrons emitted in "inelastic" reactions, e.g., (n,n'), (n,2n), (n,3n), etc. Then, the product of the cross section and the number of neutrons emitted is stored in the appropriate place in the output table (TAB array).

ADE

This routine is called by OVER13 to add energy points to the output mesh at energies below the lower bound of the resonance range, and by ADX to add points above the upper bound of the resonance range. ADE calls subroutine XLIN as points are added in order to assure that cross sections placed in the output table may be interpolated linearly with an accuracy given by input criterion EPSI.

XLIN

As stated above, this routine is called by ADE to assure that cross sections stored in the output table may be interpolated linearly with given accuracy. Cross sections at the bounds of an interval are transmitted to the routine through COMMON while the interpolation index appears in the parameter list. The cross

section, designated SIGLIN, calculated at the midpoint of the interval by linear interpolation between the bounds, is compared to the cross section computed by use of the given interpolation scheme. If the two quantities agree within input criterion EPSI, the energy and cross section at the upper bound of the interval are stored in the output table and control returned to the calling program. Otherwise, that energy and cross section are held in memory for later use, then the lower half-interval is divided in two, and the procedure is repeated until the two quantities agree within EPSI.

ADX

This routine is called by OVER13 to add smooth and resonance cross sections on an existing energy mesh, or to establish the mesh above the resonance range before performing the addition. A call is made to ADE for the addition of points to the smooth cross section table that are required in order to assure linearity. Then when energies below EUP, the upper bound of the problem being run, have been established, a call is made to MERGET to form the composite cross sections.

Existing cross sections are read from logical tape NTAPR and added to smooth cross sections already in memory and transmitted through COMMON. When NUMWD energies and composite cross sections have been stored in the output TAB array, or no more cross section records exist on NTAPR, the composite tables are written on logical unit NTAPW by a call to RITRC.

NTERP

This routine is called to determine the interpolation scheme in a particular interval of the smooth cross section table. Then a call to NTERPL with the proper index yields the cross section at the desired energy which is to be added to an existing cross section, and stored appropriately in the TAB array.

2.4.1.4 OVER14

After composite cross sections have been generated for the entire energy range desired, this routine, the main program of overlay 4, is called to reorder the tables. In the input tables to OVER14, each energy point is followed, in order, by the corresponding absorption, scatter and inelastic cross sections, and the fission cross section (or the "excess" multiplicity, the sum of the products of number of emitted neutrons and "inelastic" cross sections minus one). Here, at each energy, the total and total scatter cross sections are calculated as well as the "excess" multiplicity. Then the table of energies stored consecutively is formed and written on logical tape 12, as well as tables of consecutive total cross sections and total scattering, inelastic scattering, and fission cross sections (or excess multiplicity). These tables are also printed by means of a call to subroutine OUTT.

OUTT

This subroutine is called by OVER14 to edit the output table of energies and cross sections, stored in order of increasing energy.

2.4.1.5 OVER15

The OVER15 program of overlay 5 reads and processes the information given in File 4 of the ENDF data tape. OVER15 governs the calculations involving the establishment of x-tables for the energies at which elastic scattering is anisotropic and by a call to subroutine ANIDIN, initiates a similar procedure for anisotropic discrete inelastic scattering. The given angular distributions may be represented either in tabulated form or as Legendre coefficients in either the laboratory or center-of-mass system, as specified by control words LTT and LCT, respectively. For anisotropic discrete inelastic scattering the x-tables are tabulated on the energy mesh prescribed by the ENDF tape for the angular distribution data. For elastic scattering, the energy mesh on which the x-tables are tabulated is determined by the (card input) flag LCHI. If LCHI>0, the energy mesh used is the mesh prescribed by the ENDF tape for angular distribution data, provided that the number of entries in this energy mesh is less than the number of energy points established for cross sections in OVER12 and OVER13. If the number of entries in the former is greater than or equal to the number of entries in the latter, or if LCGI≤0, the x-tables are tabulated on the same energy mesh used for tabulating cross sections ("output", or "basic" mesh). In the discussion that follows, LCHI is assumed to be less than zero (corresponding to the basic mesh option). For LCHI>0, the procedure is similar, except that energy interpolation is bypassed.

Tests are made to determine the input energies E_1 and E_2, at which the anisotropic distribution data are given, which bracket a given entry E in the output energy table. The distributions at E_1 and E_2 are computed on the same angular mesh of 201 equally

spaced points utilizing the given interpolation scheme. If the data are given in the laboratory system, conversion to the center-of-mass system is first made by subroutine CONVT1 since the EDT requires angular data in the latter system. However, no change is made in the interpolation scheme. Then the distribution is set up at the desired output energy, employing the prescribed energy interpolation scheme. Integration under the distribution curve by means of a call to subroutine GRATE yields a table of area vs. angle for use in computing the equiprobable angles. The final step prior to initiation of the x-table computing sequence is to compute a (card input) number L moments for the 201 point distribution at E by a call to subroutine MOMENT. The first moment is compared to the average cosine computed for the distribution at the preceding energy mesh point and both values are flagged if the absolute difference exceeds 0.3.

In the case of Legendre coefficient data, coefficients at the desired output energy are calculated by use of the given interpolation scheme. The order of the Legendre expansion is taken to be the larger number of the two given at the bracketing energies. Higher order coefficients not explicitly given are taken to be zero. First order coefficients at succeeding energy points are compared and flagged in a manner similar to the procedure for tabulated data. If the coefficients are given in the laboratory system, conversion to the center-of-mass system is performed in subroutine CONVT. Values of the distribution are subsequently

computed at 201 points equally spaced in the cosine of the scattering angle. In addition, values of the area under the distribution curve are computed at these points. Linear interpolation is assumed to be valid between the 201 points generated.

At this stage, the procedures for tabulated data and coefficient data merge with a call to subroutine CALCHI, the main subroutine of the x-table computations. Each x-table which satisfies the criteria for generation of x-tables is subsequently written on logical tape 12, when all output energies have been treated, for later use in generating the EDT.

CONVT1 (ENTRY CONVT2)

CONVT1 is called by OVER15 to convert elastic tabulated angular distribution data at E_1 and E_2 from the laboratory system to the center-of-mass system. This conversion is made utilizing the relationship:

$$\mu_c = \frac{1}{A}\left[\mu_\ell^2 - 1 + \mu_\ell\sqrt{\mu_\ell^2 - 1 + A^2}\right]$$

$$p(\mu_c) = p(\mu_\ell)\left[\frac{A\sqrt{\mu_\ell^2 - 1 + A^2}}{A^2 + 2A\mu_c + 1}\right]$$

A similar conversion procedure is followed for discrete level tabulated angular distribution data beginning at ENTRY CONVT2; this entry point is called from TABU. The basic difference between the procedures for elastic and inelastic scattering is that the inelastic conversion is energy dependent. The same relationships are used

as for elastic conversion, except that A is replaced by an energy dependent effective weight $\bar{A}$ given by

$$\bar{A} = A\sqrt{1-\frac{Q(A+1)}{EA}}$$

where Q is the level excitation energy. Prior to conversion, the first μ_ℓ (algebraically smallest, usually -1) is tested to see if the condition

$$\bar{A}^2+\mu_\ell^2>1$$

is satisfied. If it is not, the tabulated value of μ_ℓ is outside the physically valid range at this energy (for example, the threshold for back-scattering in the lab is $\frac{QA}{A-1}$)[7]. In this case, an appropriate message is printed and conversion is bypassed.

<u>GRATE</u>

This routine is called to integrate the distribution curve, yielding a table of area versus μ for use in computing the equiprobable μ values. If we define g_1 and g_2 to be the magnitudes of the distribution at abscissas x_1 and x_2 (angles in the present case), and A_1 and A_2 to be the areas under the distribution curve integrated from the lower bound x_0 to x_1 and x_2, respectively, then the following equations may be written for A_2,

$$\left(A_2 = \int_{x_1}^{x_2} g \; dx \right)$$

in the case of the five possible interpolation schemes:

1. g is constant

$$A_2 = A_1 + g_1(x_2-x_1) \tag{23}$$

2. g varies linearly with x

$$A_2 = A_1 + (g_1+g_2)\,\frac{(x_2-x_1)}{2} \tag{24}$$

3. g varies linearly with ln x

$$A_2 = A_1 + g_2x_2 - g_1x_1 - \frac{(g_2-g_1)(x_2-x_1)}{\ln \frac{x_2}{x_1}} \tag{25}$$

4. ln g varies linearly with x

$$A_2 = A_1 + \frac{(g_2-g_1)(x_2-x_1)}{\ln(g_2/g_1)} \tag{26}$$

5. ln g varies linearly with ln x

$$A_2 = A_1 + \frac{g_1x_1}{a+1}\left[\left(\frac{x_2}{x_1}\right)^{a+1} -1\right], \quad a \equiv \frac{\ln(g_2/g_1)}{\ln(x_2/x_1)} \tag{27}$$

CONVT

This routine is called by OVER15 and LEGEN to convert Legendre coefficients given in the laboratory to the center-of-mass system using the energy-independent transformation matrix U^{-1} read from the ENDF data tape, i.e.,

$$f_{\ell}^{c.m.}(E) = \sum_{m=0}^{NM} U^{-1}_{\ell m}\, f_m^{lab}(E) \tag{28}$$

ANTERP

This subroutine performs the inverse interpolation to determine the equiprobable μ values (or energies as in OVER16) corresponding to given areas under the distribution curve utilizing the prescribed interpolation schemes. If the quantities defined in Section 2.4.6 are used, the relationships between abscissa x at area A bounded by A_1 and A_2 may be written as follows:

1. g is constant

$$x = x_1 + \frac{(A-A_1)}{g_1} \tag{29}$$

2. g varies linearly with x

$$x = x_1 + \frac{(A-A_1)}{\frac{g_1+g_2}{2}}, \text{ if } \frac{dg}{dx} \equiv \frac{g_2-g_1}{x_2-x_1} \leq 10^{-4} \tag{30}$$

and since

$$A = A_1 + \left(\frac{g_1x_2-x_1g_2}{x_2-x_1}\right)(x-x_1) + \left(\frac{g_2-g_1}{x_2-x_1}\right)\left(\frac{x^2-x_1^2}{2}\right), \tag{31}$$

$$\text{if } \frac{dg}{dx} > 10^{-4},$$

$$x = -\frac{d_1}{2c_1} \pm \sqrt{\left(\frac{d_1}{2c_1}\right)^2 - \frac{A-A_1}{c_1} + \frac{d_1x_1}{c_1} + x_1^2} \tag{32}$$

where

$$d_1 \equiv \frac{g_1x_2-x_1g_2}{x_2-x_1}$$

and

$$c_1 \equiv \tfrac{1}{2}\left(\frac{g_2-g_1}{x_2-x_1}\right) .$$

The sign utilized in Eq. 32 is determined by the restriction $x_1 < x < x_2$.

For the last three possible interpolation schemes, an iterative procedure is followed to solve the equations for x. If no singularities occur, areas are calculated by function subprogram AR at estimated values of x. Possible singularities occur when x_1 or x_2 equals zero, or g_1 equals g_2. If x_1 or x_2 equals zero, the value is replaced by $(\pm 10^{-10})$*, and the above procedure is followed; if g_1 equals g_2, the distribution is treated as constant.

AR

This function computes the area between x_1 and x, transmitted as an argument, for the three interpolation schemes involving logarithmic variation.

1. g varies linearly with ln x

$$A = A_1 + g_1\ (x-x_1) + \frac{g_2-g_1}{\ln\left(\frac{x_2}{x_1}\right)}\left[x \ln\ (x/x_1)-(x-x_1)\right] \quad (33)$$

2. ln g varies linearly with x

$$A = A_1 + \frac{g_1(x_2-x_1)}{\ln(g_2/g_1)}\left[\left(\frac{g_2}{g_1}\right)^{(x-x_1)/(x_2-x_1)} -1\right] \quad (34)$$

* The choice of sign is governed by the requirement that the ratio x_2/x_1 be positive (see Eqs. 25 and 27).

3. ln g varies linearly with ln x

$$A = A_1 + \frac{g_1 x_1}{a+1}\left[\left(\frac{x}{x_1}\right)^{a+1} - 1\right], \quad a = \frac{\ln(g_2/g_1)}{\ln(x_2/x_1)} \tag{35}$$

These equations are generalizations of Eqs. 25 through 27.

ANIDIN

This subroutine governs the processing of discrete level angular distributions. It is called by OVER15 when elastic scattering angular distributions have been processed.

Its supervisory roles include: initiating the reading of TAPE10 by a call to INIT; initiating calculation of 201 point distribution tables via calls to LEGEN or TABU, if Legendre coefficients or tabulated data are given, respectively; generating x-tables via calls to CALCHI and MOMNTX; and reorganizing and storing the x-tables by calling RESTOR and ENCORE (an entry point in RESTOR).

CALCHI

This subroutine, called by OVER15 and ANIDIN, calculates a table of x values and concurrently compares the "x-distribution" with the given distribution in accordance with the "α-criterion", as discussed in Section 2.3.3.

INIT

This subroutine initiates the reading of file 4 ENDF for discrete angular distributions. It skips any section which does not correspond to a level excitation by calling SKIP and senses

the file end (FEND) card, which signals the end of angular distribution data.

IOAWDIN

This subroutine reads the last card from INPUT which sets the logical variable DEBUG. DEBUG either allows or suppresses debug printout. The remainder of the operations in this routine involve printing descriptive information for discrete level angular distributions, such as the excitation energies for the given reactions.

IOFIL4

This is an auxiliary I/O routine called by OVER15. The input to this routine establishes the criteria to be used in the chi table computations, as discussed in Section 2.3.3. An input of one blank card establishes the default set of criteria (see discussion in Section 2.3.3):

(1) N is a non-decreasing function of energy;

(2) $\varepsilon_{\ell} = 0.02$, $\ell = 1,3$

(3) $\alpha = 0.5$;

(4) LADHOC = 30;

LEGEN (ENTRY LEGE)

This subroutine is called in ANIDIN to generate the angular distribution at 201 equally spaced cosines from the given Legendre coefficients at the first energy mesh point. Entry LEGE is called for given energy mesh points after the first. The calculations performed are similar to the procedure used for elastic scattering in OVER15.

MOMENT

This subroutine computes L moments for an angular distribution tabulated at 201 points. It uses trapezoidal integration and the following properties of Legendre polynomials[8]

$$P_{n+1}(x) = \frac{(2n+1)xP_n(x) - nP_{n-1}(x)}{n+1} \qquad (n \geq 1)$$

$$P_n(1) = 1, \; P_n(-1) = (-1)^n$$

MOMNTX

This subroutine computes L moments for a chi distribution of N entries and performs the ε_ℓ comparison with the moments of the given angular distribution. In addition to the properties of Legendre polynomials used in MOMENT it uses the property[8]

$$P'_{n+1}(x) - P'_{n-1}(x) = (2n+1) \, P_n(x), \qquad (n \geq 1)$$

RESTOR (ENTRY ENCORE)

This subroutine, called by ANIDIN, reorganizes and stores level chi data for each discrete reaction (MT). Entry ENCORE is called by ANIDIN when all MT have been processed, whereby the arrangement for all level chi data is finalized and stored on TAPE16. This information is subsequently read in program SETDAT when the EDT is written.

TABU

This subroutine is called in ANIDIN to generate the angular distribution at 201 equally spaced cosines from the given tabulated data. It is analogous to subroutine LEGEN, which processes Legendre data.

2.4.1.6 OVER16

This routine, the main program of overlay 6, reads and processes the information given in File 5 of the ENDF data tape, and establishes the tables required by the SAM-F EDT for the reactions designated as inelastic. Earlier the data representations treated in OVER16 were listed in Table 6. For discrete levels subroutine TPREP proceeds to read the $\sigma(E)$ vs E table from logical unit 17 (written earlier in OVER13) and, by calling subroutine SETUP, establishes the table of cross sections of level k on the output energy mesh. As each level is processed, the cumulative sum of these cross sections is written on logical unit 14 in order to conserve memory. When all the discrete levels have been treated, the data on tape 14 are read, transposed, and written on logical unit 11 as one record of LPLEV words at each output energy. The I^{th} entry is the cumulative cross section of the first I levels. The required excitation cross sections are written on tape 12 for later use in generating the EDT. If data for MT=91 was written on logical unit 17 in OVER13, a call to subroutine UPREP establishes this data on the output (or "basic") energy mesh.

For continuous spectrum components the probability distribution p(E) is read, and established on the output energy mesh. Inelastic cross sections are read from tape 15, with the implicit assumption that the order of reaction types having data on tape 15 is the order in which energy distribution data for inelastic reactions are presented in File 5. For MT=91, the inelastic cross sections are read from logical unit 17 where they were stored by subroutine UPREP. The product of cross section, p(E), and number of neutrons emitted in the reaction is formed, and the cumulative sum of this quantity over all continuous spectrum components is stored in the TAB array at each output energy. The array is used later in generating the equiprobable energy tables. If necessary, as in the case of control word LF equal to 5 or 9, the nuclear temperature $\theta(E)$ table is read and established on the output energy mesh, again by a call to SETUP. Then the distribution is either read (LF=4,5) or computed from the known expression (LF=7, 8 or 9), and at each output energy E is tabulated at 201 equally spaced points, from 0 to energy E. The table is formed in subroutine DIST (DISLF1 if FL=1 or DISLF3 if LF=3) where it is written on tape 14 for processing after all continuous distributions have been tabulated. At that point, the sum appearing in the numerator of Eq. 21, Section 2.3.4,

$$\sum_k \sigma_k^{in}(E) n_k \sum_\ell p_\ell(E) f_\ell(E \rightarrow E')$$

is calculated at each energy, E, from the data on tape 14. The cumulative distribution is normalized, as in Eq. 21, and written on tape 15. With the distribution available at each output energy, subroutine EQUIPE is called to generate the equiprobable scattered-energy tables. That is, each distribution curve is integrated, and by means of inverse interpolation in the area vs scattered energy (E') tables, the equiprobable energies E' are computed. These ENN tables, as they are described in Section 2.3.4, are then written on logical unit 12, and the tables of indices IENN and IPLEV are written on tape 14 for later use in creating the EDT.

SETUP

This routine is called to establish the cross section $\sigma(E)$, or the fractional contribution, p(E), or nuclear temperature, $\theta(E)$, arrays on the output energy mesh. The results, obtained by use of the prescribed interpolation in the input tables, are stored in appropriate places in the TAB array. Values of indices IENN and IPLEV are properly set, as is a counter for the location of the first output energy at which there is (discrete or continuous) data.

DIST

At each output energy E, this routine establishes a table of distribution g(E') at 201 points equally spaced in energy from 0 to E, given the particular representation (LF) of the distribution. For the general evaporation spectrum that is tabulated (LF=4,5), the prescribed interpolation is performed in the calculation of values at desired energies. For the Maxwellian spectrum, use is made of the relationship

$$\int_{x_1}^{x_2} g(x')dx' = \int_{E_1}^{E_2} \frac{g(E'/\theta)}{\theta} dE' \tag{36}$$

where $(x') = E'/\theta$,

$$g(x') = x'e^{-x'},$$

to set up the quantity $g(E')/\theta$, since the numerical integration performed in subroutine EQUIPE extends over energy. The 201-point table is written on tape 14 for later use in OVER16 in the generation of the composite continuous distribution due to several reaction types.

DISLF1

At each energy E, this routine establishes a table of distribution g(E') at 201 points, equally spaced in energy from 0 to E, for an arbitrary tabulated function (LF=1). This routine is analogous to subroutine DIST, which processes the other secondary energy (LF) distribution laws.

DISLF3

At each energy E, this routine establishes a table of distribution g(E') at 201 points, equally spaced in energy from 0 to E, for a discrete level excitation (LF=3). The delta function is represented as a triangle, spanning 3 points (2 if at either end of the range), such that it peaks near E' and its normalization is internally consistent.

EQUIPE

This routine is called by OVER16 to generate the equiprobable energy tables for the composite continuous energy distribution. The program numerically integrates the distribution curve, given at 201 equally spaced energy points, with the reasonable assumption that

the distribution varies linearly with energy between tabulated points. The table of area vs energy is transmitted, via the TAB array in COMMON, to subroutine EQUE which generates the equiprobable scattered-energy values and returns control to EQUIPE. At that point, the table of equiprobable energies is written on tape 12 for later use in generation of the EDT.

EQUE

Given the table of area under the distribution curve vs energy, this routine computes each of the LENN equiprobable scattered energies corresponding to particular values of area by means of a call to subroutine ANTERP. The energies are stored in the TAB array for transmission to EQUIPE.

2.4.1.7 OVER17

This routine is the main program of overlay 7 in which the EDT is generated in the format required by SAMCE.

RITEDT

Due to core storage limitations, only LENTAB words have been allotted to the TAB array. (See Section 2.8) If, during the generation of the EDT, the data to be written exceed LENTAB words, this subroutine is called each time LENTAB words have been stored. Records of 5.0 words are written on the EDT before control is returned to SETDAT to continue storing output data in the TAB array

2.4.2 PEND (OVER20)*

PEND is the controlling program of the photon production processor, the second primary overlay of SAM-X. It controls the calls to the processing subroutines, which perform all the calculational and I/O functions. The starting point for the processing procedure is determined by the variable ISTART, which is read by the card input routine CARDIP. Any abnormal start presupposes the availability of the required information on the restart tape (TAPE 14), as precomputed and stored by a previous execution of PEND. The details of this and other user options are given in the following descriptions of the routines which are loaded with PEND.

CARDIP

This routine, called by PEND, reads all the user card input concerning the processing of photon production ENDF files.

The following items are read in (user supplied) or internally set by default (for card input formats see Section 2.5):

(a) A TITLE card is read and printed.

(b) The element identifier IDN is read and printed.

(c) A flag ISTART is read and printed, the values and and corresponding implications are:

ISTART	IMPLICATION
0 (or blank)	normal start
1	restart point 1 - processing previously completed through call to TAPIN;

ISTART	IMPLICATION
2	restart point 2 - processing previously completed through call to SAVE;
3	restart point 3 - processing prevoiusly completed through call to FILE15;

For ISTART>0, a restart tape must be available (designated as TAPE 14) from a previous execution of PEND. The auxiliary restart tape (TAPE 11) must also be available if ISTART=3 and FILE14 data was processed.

(d) ISCAN(10) is read and printed. Currently, only the first 6 entries are operational. This array presets a 3-way flag (ISCANA) at 6 milestones in the complete execution of PEND. For ISCANA<0, execution is terminated; ISCANA=0, execution continues, but intermediate calls to DSPLAY are suppressed; ISCANA>0, execution continues with calls to DSPLAY. The 6 positions corresponding to the first 6 entries in ISCAN are:

ISCAN(I)	MILESTONE
(1)	precedes call to DICT
(2)	precedes call to SMOOTH
(3)	precedes call to FILE 12
(4)	precedes call to FILE 13
(5)	precedes call to FILE 15
(6)	precedes call to TAPOUT

The ISCAN≠0 option is normally not employed, but it does provide the flexibility of selective displays, both on the original execution and on restarts.

(e) Next, a variable MIDE is read, which designates the number of "photons" to be discretized from the continuous photon distributions (if any). If MIDE$\leq$0, a default set of photons is established as follows:

(1) the number of discretized photons is set to 41;

(2) the spectrum range from 0. to 10^8 ev is subdivided into 41 integration intervals, or "bins," with a low energy bin (0.0, 0.25 Mev) defined for a photon of energy 0.125 Mev, 39 bins of width 0.5 Mev between 0.25 and 19.75 Mev defined for photon energies at the respective bin midpoints, and a catchall bin (19.75, 100.0) Mev defined for a photon of energy 20.0 Mev. On option, these default values may be superseded by user supplied energy and bin definitions for up to 99 photons.

(f) Finally, the criteria for processing photon angular distributions (FILE 14) are read in. These criteria are described in Section 2.3.3.

PKIP

This routine, called by PEND, SMOOTH, FILE14, and FILE15, is the same as the SKIP routine of program NUTRON.

DICT

This routine, called by PEND, examines the dictionary of ENDF File 1 and establishes the processing sequence of subsequent files. In particular, DICT keeps track of all the reactions (MT numbers) appearing in File 12, so that the corresponding neutron cross sections are extracted from ENDF File 2 and/or File 3.

TAPIN

This routine is called by PEND to retrieve the basic neutron energy mesh and corresponding non-elastic cross sections from the NEDT. The energy mesh is extracted directly; the non-elastic cross sections are computed from the total, total scattering, and total inelastic scattering cross sections.

Tape NEDT (assigned to logical TAPE 13) is searched for the desired element IDN. Once this EDT is found, it is combed (as directed by the relevant pointers) until the energies, total, scattering, and inelastic cross sections have been stored contiguously in the TAB array, starting in TAB(1) and ending in TAB(3*NEN+NI), where NEN is the length of the energy table and NI(≤NEN) is the number of inelastic entries. The final step in this procedure, based on the expression $\sigma_{ne} = \sigma_t - \sigma_s + \sigma_{in}$, computes the non-elastic cross sections in TAB(NEN+1) through TAB(2*NEN).

PARAM

Currently, this skeleton routine will STOP execution if called by PEND. Ultimately, this routine will be designed to process ENDF File 2 in order to compute the cross sections, which must be combined with the ENDF File 12 yields when applicable. (If resonance parameters are not given in File 2, only the smooth cross sections of File 3 are applicable.)

SMOOTH

This routine is called by PEND if File 12 information is given (as sensed by DICT). For each MT appearing in File 12, this routine processes the corresponding neutron cross sections in File 3

by calling SUBROUTINE STBLSH. All other MT numbers in File 3 are bypassed by calling PKIP(3).

After each call to STBLSH, the NEN smooth cross sections, tabulated on the basic mesh, are stored on tape NPDT for subsequent calculations in FILE12. Also, if the display switch is on (ISCANA>0), a call to DSPLAY prints the smooth cross sections.

STBLSH

This routine, called by both SMOOTH and FILE15, sets up an ENDF TAB1 array on the basic energy mesh, utilizing the specified ENDF interpolation rules. Interpolation is accomplished by a call to PTERPL.

PTERPL

This routine, called by DSCRT, STBLSH, FILE15, TABLE, and INTEG, is the same as the NTERPL routine of program NUTRON.

FILE12

This routine, called by PEND, controls the processing of ENDF File 12 multiplicities (option LO=1). The current version of FILE12 cannot treat transition probability arrays (option LO=2) and execution is terminated, after printing LO and MT, for LO≠1.

For each MT value in File 12, the NK discrete photons (and possibly one photon continuum) is processed by a call to SUBROUTINE DSCRT.

DSCRT

This routine, called by FILE12 and FILE13, computes yields on the basic energy mesh. The ENDF specified interpolation rules

are utilized in calling PTERPL. In addition, DSCRT notes the first and last mesh point for which an entry is greater than 10^{-9} and temporarily stores discrete entries on tape NSDT and continuum entries on tape NDFC. If the display switch is on, a call to DSPLAY prints the computed arrays.

SKIPTB

This routine, called by FILE12 and FILE13, skips the first TAB1 record in each section of ENDF File 12 and File 13 for which NK>1. (If the total number of discrete photons and photon continua is one, i.e., NK=1, this TAB1 record, which tabulates the total yield for a given reaction, is omitted.) It is also called from FILE15 to "flip" past unused TAB1 records.

FILE13

This routine, called by PEND, controls the processing of ENDF File 13 photon production cross sections, in a manner completely analogous to the procedure in FILE12 under option LO=1.

PAVE

This routine, called by PEND, saves on restart tape NPDT the information temporarily stored on NSDT and NDFC by DSCRT. An additional function performed by PAVE is the sorting, in ascending MT order, of the continua arrays written to NPDT. These arrays are subsequently combined with the information in File 15, which is given in ascending order of MT by ENDF. Since continua arrays may derive from File 12 and/or File 13, the ascending MT order might not have been preserved without sorting.

FILE14

This routine, called by PEND, governs the processing of photon angular distributions in ENDF File 14.

LEGEND

This subroutine is called by FILE14 to generate an angular distribution at 201 equally spaced cosines for one energy mesh point if Legendre coefficients are supplied by ENDF. It is similar to the LEGEN routine of program FILE4.

TABLE

This routine, called by FILE14, performs the same function as LEGEND, when ENDF gives angular distributions in the form of tabulated data.

POMENT

This routine, called by TABLE, is the same as the MOMENT routine of program OVER15.

PALCHI

This routine, called by FILE14, is the same as the CALCHI routine of program OVER15.

PNTERP

This routine, called by PALCHI, is an abbreviated version of the ANTERP routine in program OVER15. It utilizes only linear interpolation.

POMNTX

This routine, called by FILE14, is the same as the MOMNTX routine of program OVER15.

RSTORE

This routine, called by FILE14 reorganizes and stores the CHI data for one photon at a time.

SAVE14

This routine, called by FILE14, completes the organization of chi data for all photons and saves this information on the auxiliary restart tape (see Tape Utilization, Section 2.7).

FILE15

This routine is called by PEND to process the continuous photon energy spectra in ENDF File 15. Before describing the processing procedure, it is useful to summarize the File 15 discussion of Ref. 10:

> File 15 provides a means for representing continuous energy distributions of secondary photons. These energy distributions, $f(E \rightarrow E_\gamma)$, have the units of ev^{-1} and are normalized such that
>
> $$\int_0^{E_\gamma^{max}} f(E \rightarrow E_\gamma) dE_\gamma = 1,$$
>
> where E_γ^{max} is the maximum possible secondary photon energy. The $f(E \rightarrow E_\gamma)$ can be broken down into the weighted sum of several different distributions, normalized to unity over $(0, E_\gamma^{max})$, viz:

$$f(E \to E_\gamma) = \sum_{j=1}^{NC} p_j(E) q_j(E \to E_\gamma) \quad (\text{ev})^{-1},$$

where NC ≡ the number of partial distributions used to represent $f(E \to E_\gamma)$.

$q_j(E \to E_\gamma)$ ≡ the jth normalized partial distribution in the units ev^{-1}.

$p_j(E)$ ≡ the probability or weight given to the jth partial distribution, $q_j(E \to E_\gamma)$.

The absolute energy distribution cross section, $\sigma_\gamma(E \to E_\gamma)$, can then be constructed from the expression

$$\sigma_\gamma(E \to E_\gamma) = \sigma_\gamma(E) f(E \to E_\gamma) \quad (\text{b/ev}),$$

where $\sigma_\gamma(E)$ is the integrated cross section for the continuum given either directly in File 13 or through the combination of Files 2, 3, and 12.

Based on the above discussion, the function of FILE15 is to compute a set of discretized photons from the expressions

$$y_{\gamma_i}(E) = Y_\gamma(E) \int_{\Delta E_{\gamma_i}} f(E \to E_\gamma) dE_\gamma$$

$$Y_\gamma(E) = \sigma_\gamma(E)/\sigma_{ne}(E)$$

where the $Y_\gamma(E)$ are the continua yields tabulated on the basic energy mesh by FILE12 and/or FILE13, and ΔE_{γ_i} is the ith integration bin specified in CARDIP. The computation for each of the NC partial distributions for a given MT proceed as follows:

First, the weight function for the partial distribution is tabulated on the basic mesh by a call to STBLSH. If the display switch is on, the tabulation is printed by a call to DSPLAY. Two successive calls to SUBROUTINE INTEG produce the first 2 sets of partial fractions by integrating the partial distributions over the bins. At basic mesh points between these two sets, the corresponding fractions are computed by the specified ENDF interpolation scheme, using PTERPL. Successive fraction sets at higher interpolation energies are computed as needed. The final step in the computation of a set of discretized photon yields is to form the cumulative product

$$y^{n}_{\gamma_i}(E_m) = y^{n-1}_{\gamma_i}(E_m) + Y_\gamma(E_m)\,p_j(E_m)\int_{\Delta E_{\gamma_i}} q_j(E_m \rightarrow E_\gamma)\,dE_\gamma$$

The above expression implies that the contributions from all NC partial distributions for all MT sections are superimposed. After each iteration, the current set of cums is written on either NSDT or NDFC, which alternate as read and write tapes during the looping over NC. When all of the MT sections of File 15 have been processed, the discretized yields are rearranged from tabulations of yields as a function of neutron energy, to tabulations as a function of discretized photon energy. This is accomplished by a call to SUBROUTINE CONFRM.

INTEG

This routine, called by FILE15, computes a set of partial fractions at a given neutron energy for the ENDF specified normalized partial distribution. Integration end points for each bin are determined by calls to PTERPL, while the integrals are computed by SUBROUTINE PRATE

PRATE

This routine, which is the same as the GRATE routine of program NUTRON, is called by INTEG to perform the integration of a distribution in accordance with the ENDF specified interpolation rules. It is also utilized by SUBROUTINE TABLE.

CONFRM

This routine is called by FILE15 to transpose the computed continuum photon yields, from photon energy tabulations (rows) to neutron energy tabulations (columns), to conform with the storage scheme of the GPDT. The objective is to limit the number of read passes of tapes N1 and N2 (N1 being the last of the two tapes, NSDT or NDFC, written on in FILE15) within the constraints of the dimension of blank common (NEMID) and the range of neutron energy mesh points (NE) for which a non-zero ($>10^{-9}$) entry exists.

The read pass of N1 has a two-fold function: determines NE and writes an abbreviated version of N1 on N2 (the second of the two scratch tapes used in FILE15) by eliminating entries outside the bounds specified by NE. The number of passes (NPASS) of N2 necessary to perform the transformation is then given by the algorithm,

NPASS = (MIDE*NE-1)/NEMID+1

where MIDE is the number of discretized continuum photon energies.

After each pass of N2, the columnar tabulations, which are stored contiguously in blank common, are written to the restart tape NPDT, one column per binary record. If the display switch is on, these columnar tabulations are printed by DSPLAY.

TAPOUT

This routine is called by PEND to retrieve the information stored on restart tape NPDT, rearrange the information in accordance with the format of a GPDT, append the necessary pointers, and write out the complete GPDT on tape NSDT (designated as TAPE15) in records of length 510 words. If the length of the GPDT exceeds the dimension of blank common (NEMID), the GPDT is written piecemeal by intermediate calls to SUBROUTINE RITPDT.

CHIOUT

This routine, called by TAPOUT, reads the chi data from the auxiliary restart tape (see Sec. 2.7) and merges it with the remainder of the GPDT.

RITPDT

This routine, called by TAPOUT and CHIOUT, writes fragments of a GPDT whenever the size of the GPDT exceeds the blank common dimension.

2.4.3 WEED (OVER30)*

WEED is the controlling program of the data reduction processor, the third primary overlay of SAM-X. It controls the calls to the processing subroutines, which perform all the calculational and I/O functions. The choice of reduction modes is governed by the integer flag IN and the flag array ISCAN controls continuation/termination of execution and also serves as a display switch. All flags are set in the card input routine CARDI2. Details of the latter routine as well as others which are loaded with WEED are given in the following descriptions.

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*See second footnote, p. 15.

CARDI2

This routine called by WEED reads all the user card input concerning the reduction in length of a GPDT.

The following items are read in (user supplied) or internally set by default (for card input formats, see Section 2.5):

(a) A TITLE card is read and printed.

(b) The element identifier IDN is read and printed.

(c) A flag IN is read and printed. For IN=1, only the weeding mode of reduction is exercised; IN=2, only the binning mode is exercised; any other value of IN effects both modes.

(d) ISCAN(3) is read. The entries in this array correspond to a 3-way flag at 3 milestones in the execution of WEED. For ISCAN(i)<0, execution is terminated; ISCAN(i)=0, execution continues, but call to DSPLAY (to display the current data) is suppressed; ISCAN(i)>0, execution continues with a call to DSPLAY. The 3 positions corresponding to the 3 values of i in ISCAN(i) are:

i	MILESTONE
1	after call to GPDIN
2	after call to GPDOUT
3	after call to BIN

(e) The weeding criterion, FACTOR, is read and printed. It is ignored if IN=2. If FACTOR=0.0 (or blank), it is reset to the default value of 0.05 (termed "standard 5% weeding"). For 0.0<FACTOR<0.001, execution is terminated.

(f) If IN≠1, the binning criteria, FAC and MEMAX, are read and printed. If MEMAX<1, it is reset to the default GPDT length 2040 (i.e., the binning continues until the GPDT length does not exceed MEMAX or only one photon energy remains). If 1≤MEMAX<510, MEMAX is reset to 510, the minimum length of an EDT, i.e., one binary record.

GPDIN

This routine, called by WEED, reads into blank common the entire old GPDT, corresponding to element IDN. When IDN is found on tape LOD (designated TAPE15) the length of this GPDT is compared with the dimension of blank common, NEMID, and execution is terminated if the number of 510 records represented by the GPDT length exceeds NEMID.

COMB

This routine is called by WEED if IN≠2. It is the main routine of the weeding mode of data reduction. The basic premise for this procedure is that the reduced set of original mesh points corresponds to the minimum number of energies sufficient to compute all of the eliminated yields (within the relative fraction FACTOR) by linear interpolation.

The reduction proceeds in a loop over the basic energies (tabulated high to low). If the mesh point being considered corresponds to an end point (first or last tabulated entry) for any photon, the mesh point is retained and becomes the new high reference point for interpolation. For intermediate mesh points, the low reference point is chosen to be the next tabulated energy, and the yield for every photon in the range is computed by linear

interpolation. As soon as the interpolated value for any photon yield effects a deviation which exceeds the allowed tolerance, the mesh point is retained, as in the case of an end point. If all the photons in the range satisfy the FACTOR criterion, the energy point being considered is tagged as a "weed" by a minus sign (it cannot be eliminated until subsequent interpolation sequences have been completed).

When all of the entries have been combed in the above manner, the actual contraction of the GPDT is accomplished in SUBROUTINE GPDOUT.

GPDOUT (ENTRY GPDTUT)

GPDOUT is called by WEED to complete the data reduction in the weeding mode. The procedure involves negating all the photon yields which correspond to energy mesh points negated in COMB (weeds), reseting all pointers for the reduced GPDT, and contracting the old GPDT by "squeezing out" all negative entries, or weeds. If IN=1 (i e., the reduced GPDT will not be binned) the reduced GPDT is written to tape NEW (designated TAPE9) in records of 510 words each, starting at entry point GPDTUT. The latter is also called by SUBROUTINE BIN.

BIN

This routine is called by WEED if IN≠1. Its primary function is to rearrange the GPDT so that photon energies are stored in ascending order, as a prelude to the actual binning procedure. Binning is initiated by a call to SUBROUTINE SARDIN. After binning has been completed, a call to GPDTUT (an entry point in GPDOUT)

causes the reduced GPDT to be written in blocks of 510 words on tape NEW.

SARDIN

This routine, along with its subordinate SUBROUTINE SQUEEZ, performs the binning or superposition of adjacent (in energy) photons. It is called by BIN after all the photons have been sorted in ascending photon energies. This order is not a format requirement of a GPDT; it just simplifies the binning procedure.

A hierarchy of conditions must be satisfied before two photons are superimposed:

(1) The photons must be adjacent in energy.

(2) The photons must have the same angular distributions.

(3) The neutron energy ranges of the photons must overlap (i.e., they must have at least one common mesh point).

(4) The two photon energies define the minimum fractional interval.

(5) The minimum fractional interval is less than the criterion FAC, or the current GPDT length is greater than the criterion MEMAX.

SQUEEZ

This routine is called by SARDIN when a photon pair has been selected by the hierarchical testing in SARDIN. SQUEEZ proceeds to establish new integer indicators, such as pointers and range delimitors, resulting from its superposition of the designated photon pair, and shifting all information so as to eliminate superseded entries. The new photon energy representing the combined pair is computed as the average of the two values.

2.4.4 GAMMA (OVER40)*

GAMMA is the controlling program of the ENDF gamma ray cross section processor, the fourth primary overlay of SAM-X. It reads a list of the elements to be processed and the logical designation of ENDF data tape to be read.** When GAMMA finds a desired element on the ENDF tape it passes control over to GELEM.

GELEM

This routine called by GAMMA reads in the total, coherent scattering, and incoherent scattering cross sections. Other reactions are bypassed.

GELEM modifies the total cross section by subtracting out the coherent scattering cross section, since the latter process is not presently treated by the SAM-F and SAM-A codes.

GELEM controls the creation of the output data tape (GEDT) on unit 16.

LINEAR

This routine adds points to the total cross section vs. energy table so that linear interpolation may be used at all times between data points.

SEEK

This routine locates the position of a given variable in a monotonically increasing array.

TERP1

This routine is used for interpolation.

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* See second footnote, p.15.

** GAMMA may read gamma ray cross section data from the ENDF neutron cross section and gamma ray production tape (unit 10), from a separate tape containing only gamma ray cross sections (unit 11), or from the card reader (unit 5).

2.4.5 BCDEAN (OVER50)*

BCDEAN is the controlling program of the two way EDT converter, the fifth primary overlay of SAM-X. It controls the calls to the processing subroutines, which perform all the calculational and I/O functions. The choice of conversion mode is governed by the sign of the problem vector ISTART (see Section 2.5.7).

BCDBIN

This routine is called by BCDEAN to perform the BCD-to-binary conversion.

BINBCD

This routine is called by BCDEAN to perform the binary-to-BCD conversion. The structure of the BCD EDT, as produced by BCDEAN, is given in Appendix N.

CLEAN

This routine is called by BCDEAN to remove all ampersands, which may have been introduced during binary-to-BCD conversion.

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* See second footnote, p. 15.

2.5 Input Description

2.5.1 Default Options

Great care has been taken to make the input to SAM-X as convenient as possible for the user.

Although SAM-X is an extremely complex code, which is able to treat a multitude of ENDF options for the presentation of data, the amount of input, necessary to run the code, has been successfully limited to just a few cards.

This was accomplished by reducing much of the input data to blank entries (i.e., default modes) which allow SAM-X to set many key parameters internally. Although these default modes may be overridden, the authors highly recommend that beginners make extensive use of the default option capabilities of the code.

The following cards are entered as input to SAM-X. (Before preparing input, the user should read Section 2.6 - Notes to the User.) Except for the initial card, which must be included for every execution of SAM-X, all the cards have been grouped, for clarity, into five sections, corresponding to the five component processors NUTRON, PEND, WEED, GAMMA, and BCDEAN respectively.

2.5.2 SAM-X (Main Overlay) Input

The input for a given execution of SAM-X comprises a single contiguous package. For example (in the input card which follows), if the execution of PEND and WEED is desired: set IA=2, IB=3 on Initial Card; omit all cards described in NUTRON, GAMMA, and BCDEAN Input, and include all cards for PEND and WEED.

Initial Card (3I1)

Item	Column	Variable	Description
1	1	IA	Designates execution entry point at NUTRON, PEND, WEED, GAMMA or BCDEAN by the values 1, 2, 3, 4 or 5 respectively.
2	2	IB	Designates execution termination after NUTRON, PEND, WEED, or GAMMA by the values 1, 2, 3, or 4 respectively.*
3	3	IC	Control variable for BCDEAN. IC=0 (or blank) will suppress BCDEAN IC=1 will activate BCDEAN in either mode depending upon IA: a) if IA=5 BCDEAN will execute BCD-to-binary b) if IA<5 BCDEAN will execute binary-to-BCD

NOTE: for IC=1 and IA<5, BCDEAN will perform its processing following each step of the SAM-X execution. Hence, the input to BCDEAN, which remains unaltered, must be inserted between the appropriate inputs for NUTRON, PEND, WEED and GAMMA.

2.5.3 NUTRON INPUT

If IA=1 (as specified on Initial Card) processing begins with NUTRON, the neutron element data processor. Processing is controlled by the input cards described in this section.

---

* If IA=5, the value of IB is ignored, i.e. execution is terminated after the BCD-to-binary conversion is completed (note description of IC).

Card #1 (4I10)

Item	Column	Variable	Description
1	1-10	NDEF	Default values flag. If zero (or blank): omit remainder of Card #1, except for MTEST, give Card #2, omit Cards #3 and #4, give Card #5, omit Card #6 (omitted variables will assume the default values specified below). A non-zero entry for NDEF requires inclusion of Cards #1 through #6.
2	11-20	NUMWD	Number of words in the energy and cross section tables that are stored in memory before being written on tape. (A blank entry yields default value = 2000.)
3	21-30	MTEST	For MT<MTEST,* printing of input cross sections for that MT value in REDTAB1 will be suppressed. (Default of zero will generate extra printout.)
4	31-40	JUNIN	Specifies method for obtaining the average unresolved resonance cross section. If JUNIN=2, the code utilizes the Gaussian quadrature method, JUNIN=1 specifies the method of MC^2. (A blank entry yields a default value of JUNIN=2.)

Card #2 (10A6)

Item	Columns	Variable	Description
1	1-60	TITLE	Hollerith description of the NUTRON problem, printed at the top of each output page (in NUTRON execution).

Card #3 (2E10.3) Omit for NDEF=0

Item	Columns	Variable	Description
1	1-10	ELO	Lower energy bound (ev) of the range on which cross sections are to be generated. (A blank yields default = 1.0E-3).
2	11-20	EUP	Upper bound (ev) of the range on which cross sections are to be generated. (A blank yields default = 1.5E+7).

---

* If 901≤MTEST≤999, scattered energy distribution printing is also suppressed. If MTEST≥1000, scattered energy distribution and output cross section printing are both also suppressed.

Card #4 (I10) Omit for NDEF=0

Item	Columns	Variable	Description
1	1-10	IMULT	Control word which, if entered as 0, indicates that fission cross section is to be calculated. Otherwise, multiplicity is to be calculated. Generation of NEDT for SAM-F requires that IMULT≠0 (multiplicity option required).

Card #5 (7E10.3)

Item	Columns	Variable	Description
1	1-10	ZAP	Identifier for desired material, appearing on the ENDF tape; equal to 1000×Z+A for an isotope of atomic number Z, atomic weight A; e.g., 92238.0 for U^{238}; equal to 1000×Z for the naturally occurring mixture of isotopes.
2	11-20	TEMP	Temperature in °K, for use in Doppler broadening resolved resonance cross sections. (A blank yields default = 293.).
3	21-30	WIDTHS	Number of total widths within which resonances contribute to the cross section at a given energy. (A blank yields default = 1000.)
4	31-40	EPSI	Value of convergence criterion used in establishment of the energy mesh in resolved resonance range at lower bound of range. (A blank yields default = 0.05.)
5	41-50	EPSJ	Value of convergence criterion used in establishment of energy mesh in the resolved resonance range at upper bound of range. (A blank yields default = 0.15.)
6	51-60	DELU	Lethargy width desired for groups in unresolved resonance range. (A blank yields default = 0.03.)
7	61-70	ECONT	Lowest energy, in ev, at which secondary energy data for the continuum are given on the ENDF data tape for reaction types treated as nonelastic continuum by NUTRON. Entry is required only if this lowest energy occurs for a reaction type other than the first nonelastic continuum type read. If lowest energy appears twice, the first time with a zero cross section, the second time with a nonzero cross section, ECONT should be a value of energy slightly higher than the lowest energy.

Card #6 (2I10, E10.3, 3I10) Omit for NDEF=0.

Item	Columns	Variable	Description
1	1-10	MTABLO	Reaction type (value of MT) whose File 3 data determine the energy mesh below the resonance range. If no resonance range exists, MTABLO determines the energy mesh below the energy break point, EN1, (see third entry of the card). Exclude MT=51 through 91. (A blank yields default = 102.)
2	11-20	MTABUP	Reaction type (MT) whose File 3 data determine the energy mesh above the resonance range. Exclude MT=51 through 91. (A blank yields default = 2.)
3	21-30	EN1	Energy, in ev, which serves as the break-point below which MTABLO determines the output energy mesh, and above which MTABUP determines the mesh, if no resonance parameters are given on the ENDF tape. (A blank yields default = ELO as specified on Card #3.)
4	31-40	LCHM	A flag, utilized in FILE 4. If entry is <1, x-tables for anisotropic elastic scattering will be established on the output energy mesh; if entry is ≥1, x-tables will be established on the input energy mesh, provided the number of input mesh points is less than the number of output mesh points; (otherwise, output mesh is used). If NDEF=0 LCHM is internally set=11.
5	41-50	LENM	Number of entries desired, at each output energy in the equiprobable scattered-energy table, for inelastic scattering. (A blank yields default = 11).
6	51-60	INTEST	Control word which, if entered as 0, indicates use of test on the absorption cross section in establishment of energy mesh in resolved resonance range. If entered as nonzero, test made on total cross section. Note, however, that if NDEF=0 (see Card #1), INTEST is set to 1.

Card #7 (2I5)

The following card is read by IOFIL4. A blank card will establish default criteria for computation of angular distribution chi tables.

Item	Columns	Variable	Description
1	1-5	LADHOC	Maximum number of chis to be computed (default value = 30).
2	6-10	L	Number of moments to be computed (default value = 3)

Card #8 (10F8.3)

This card must be omitted if Card #7 is blank (default values desired). Otherwise, this card is repeated until L entries (as specified on Card #7) have been read.

Item	Columns	Variable	Description
1	1-8	EPS(1)	Maximum allowed deviation in first moment (default value = 0.02)
2	9-16	EPS(2)	Maximum allowed deviation in second moment (default value = 0.02)
3	17-24	EPS(3)	Maximum allowed deviation in third moment (default value = 0.02)
4	25-32	EPS(4)	Maximum allowed deviation in fourth moment
⋮	⋮	⋮	
10	72-80	EPS(10)	Maximum allowed deviation in tenth moment.

Card #9 (E12.4)

This card must be omitted if Card #7 is blank (default value desired).

Item	Columns	Variable	Description
1	1-12	ALPHA	α-criterion (see discussion in Section 2.3.3). (default value = 0.5).

Card #10 (L1)

This card is normally left blank (debug printout suppressed).

Item	Columns	Variable	Description
1	1	DEBUG	A T punched in column 1 produces debug printout; an F (or blank) suppresses debug printout.

> If BCDEAN is being invoked, in the binary-to-BCD mode, enter BCDEAN input (Section 2.5.7) here.

2.5.4 PEND INPUT

The details of user supplied PEND input are elaborated in Section 2.4.2.

Card #1 (20A4)

Item	Columns	Variable	Description
1	1-80	TITLE	Hollerith description of the PEND problem.

Card #2 (2I10)

Item	Columns	Variable	Description
1	1-10	IDN	Fixed point identifier for desired material (see analogous floating point description for ZAP, NUTRON Card #5).
2	11-20	ISTART	(See discussion in description of CARDIN, the first routine of Section 2.4.2.) A blank entry (default option) implies normal start.

Card #3 (10I5)

Item	Columns	Variable	Description
1	1-5	ISCAN(1)	(See discussion in description of CARDIN, the first routine of Section 2.4.2.) A blank card (default option) implies normal execution.
2	6-10	ISCAN(2)	
⋮	⋮	⋮	
10	46-50	ISCAN(10)	

Card #4 (I5)

Item	Columns	Variable	Description
1	1-5	MIDE	Number of photons discretized from continuous photon distributions. A blank entry (default option) yields a default set as described in description of CARDIN routine, the first routine of Section 2.4.2.

Card #5 (6E12.4)

This card must be omitted if Card #4 is blank (which establishes a default set of discretized photons and integration "bins"). Otherwise, for 0<MIDE≤99, MIDE photon energies may be specified (repeating the foramt of Card #5 for [(MIDE-1)/6] +1 cards) followed by the corresponding (MIDE+1) integration bin specifications (repeating the format of Card #5 for MIDE/6+1 cards).

Cards #6,7,8

The next three cards for PEND input are identical to Cards 7-9 of NUTRON.

If BCDEAN is being invoked in the binary-to-BCD mode, enter BCDEAN input (Section 2.5.7) here.

2.5.5 WEED INPUT

The details of user supplied WEED input are elaborated in Section 2.4.3.

Card #1 (20A4)

Item	Columns	Variable	Description
1	1-80	TITLE	Hollerith description of the WEED problem.

Card #2 (E10.3, 5I5)

Item	Columns	Variable	Description
1	1-10	FACTOR	Weeding criterion (ignored if IN=2). A blank entry yields default = 0.05 (i.e.,"standard 5% weeding").
2	11-15	IN	Weeding/binning mode flag. IN=1 implies weeding only, IN=2, binning only; any other value yields both modes. Default mode is a blank entry.
3	16-20	IDN	Material identifier (same as item 1, Card #2 for PEND).
4	21-25	ISCAN(1)	(See discussion in Section 2.4.3.) Blank entries (default option) yield normal execution.
5	26-30	ISCAN(2)	
6	31-35	ISCAN(3)	

Card #3 (E10.3, I5)

This card is necessary only if IN$\neq$1.

Item	Columns	Variable	Description
1	1-10	FAC	Binning criterion (usually set = 0.04).
2	11-15	MEMAX	GPDT length criterion. A blank yields default = 2040.

> If BCDEAN is being invoked in the binary-to-BCD mode, enter BCDEAN input (Section 2.5.7) here.

2.5.6 GAMMA Input *

Card #1 (3I10)

Item	Columns	Variable	Description
1	1-10	NUMELM	Number of elements to be processed.
2	11-20	N	File containing ENDF data: =5 for card reader; =10 for tape containing neutron and; gamma ray production data also; =11 for tape containing only photon data; A blank yields default=11.
3	21-30	IDBUG	=0 do not display the generated GEDT; =1 do display the generated GEDT.

Card Set #2 (7E10.3)

These cards give the elements to be processed. There are seven entries per card with a total of NUMELM entries. Each element is identified as a floating point number equal to 1000xZ+A (where Z is the atomic number; A the atomic weight) for a single isotope, or 1000xZ for a naturally occurring mixture of isotopes.

If the ENDF data are being read in by the card reader, such data now follows Card Set #2. Be sure to include one initial card which corresponds to the "header" card of an ENDF tape.

If BCDEAN is being invoked in the binary-to-BCD mode, enter BCDEAN input (Section 2.5.7) here.

* Please see important "Note to the User" on the following page.

Note to the User

It is important to note that coherent scattering is presently not treated by SAM-F or SAM-A. Hence incoherent scattering is the only scattering process considered and the total cross section is adjusted accordingly. Klein-Nishina formulation is used for the scattering. The present treatment of scattering, which will be upgraded to treat coherent scattering in the immediate future, becomes increasingly poor as it approaches the X-ray region. Hence, SAM-CE is presently not applicable to most X-ray studies.

2.5.7 BCDEAN Input

Card #1 (I3)

Item	Columns	Variable	Description
1	1-3	ISTART	Problem vector, whose magnitude is the number of materials to be converted, and whose sign indicates direction of conversion: -1, binary-to-BCD; ≥1, BCD-to-binary.

The remaining cards are repeated, in groups, for each of the |ISTART| materials.

Card #2 (2I5,1X,I4)

Item	Columns	Variable	Description
1	1-5	ID	Fixed point element identifier, equal to ZZAAA.
2	6-10	IT	For ISTART=-1 only: Number of descriptive text cards to be appended to BCD version of the EDT. IT>1. (Leave blank for ISTART≥1)
3	12-15	MAT	Arbitrary material identifier (intended to correspond to ENDF MAT#). May be left blank if any MAT# for a given ID will suffice.

The next card is repeated IT times, provided ISTART =-1.

Otherwise, it is omitted.

Card #3 (17A4, A2)

Item	Columns	Variable	Description
1	1-70	TITLE	Descriptive text to be appended to BCD version of the EDT.

2.6 Notes to the User

1. Core storage limitations require that generated data tables be dumped on tape after NUMWD words have been stored in memory. Generally NUMWD is entered as 2000 but can be increased to 5000 if File 3 data table for all reaction types is small (~200 entries). An excessively small value of NUMWD will result in greatly increased tape handling time in the code.
2. Input quantities TEMP, WIDTHS, EPSJ are used by NUTRON only if resonance parameter data are given on the ENDF tape. If such is the case, note that temperature dependence for the resolved resonance range only is treated. Generally, WIDTHS is entered as 1000. The convergence criterion varies logarithmically with energy in the resolved resonance range, from EPSI at the lower bound to EPSJ at the upper bound. EPSI is generally entered as 0.05 and EPSJ as 0.15, in order to keep running time reasonable.
3. Even if no resonance parameter data are given, EPSI is the accuracy within which generated cross sections vary linearly with energy.
4. To establish values for MTABLO and MTABUP, the user should examine the File 3 data to determine reaction types for which the most detailed description is given below and above the prescribed resonance range. If no resonance range is defined, one should examine cross section variation at low and high energies (and thus determine EN1). Generally, MTABLO=102 (capture), and MTABUP=2 (elastic scattering).

Note that the inelastic partials (MT=51,52,...,91) must not be entered for either MTABLO or MTABUP.

5. Experience in using NUTRON has indicated the default criteria for computing angular distribution chi tables to be entirely adequate for most applications. Hence a blank for Card #7, omission of Cards #8 and #9, and a blank for Card #10 is suggested.

6. Due to voluminous printout, processing has been restricted to one material per execution (except for program GAMMA).

7. The interdependence of NUTRON, PEND, WEED, GAMMA, and BCDEAN is such that the NEDT (for a given material) produced by NUTRON is required input for PEND; the GPDT (for a given material) produced by PEND (or a previous execution of WEED) is required input for WEED; a GEDT is produced independently by GAMMA; and a BCD EDT, produced by BCDEAN, requires a binary EDT from one (or more) of the first four processors. Hence, although execution of SAM-X may begin with NUTRON, PEND, WEED, GAMMA, or BCDEAN as specified on the Initial Card, the input tape prerequisites must be satisfied (see Section 2.7 for specific tape assignments).

2.7 Tape (File) Utilization

NUTRON

Logical Unit	Description
5	Standard card input.
6	Standard printed output.
10	ENDF input.
13	Neutron element data tape (NEDT) generated from ENDF.
9,11,12,14,15, 16,17	Scratch files (unit 12 is equivalenced to unit 9).

PEND

Logical Unit	Description
5	Standard card input.
6	Standard printed output.
10	ENDF input.
13	NEDT generated by NUTRON (required input).
14	Restart tape.
11	Auxiliary restart tape.
15	Gamma production data tape (GPDT) generated from ENDF.
12	Scratch file.

WEED

Logical Unit	Description
5	Standard card input.
6	Standard printed output.
15	GPDT generated by PEND, or by a previous execution of WEED (required input).
9	GPDT generated in current execution of WEED.

GAMMA

Logical Unit	Description
5	Standard card input.
6	Standard printed output.
10	ENDF input (if same tape as for NUTRON or PEND).
11	ENDF input (if separate gamma ray cross section data tape).
16	Gamma ray cross section element data tape (GEDT) generated from ENDF.

BCDEAN

Logical Unit	Description
(binary-to-BCD mode)	
4	Output EDT; BCD format
5	Standard card input
6	Standard printed output
9	Input GPDT (from WEED); binary
13	Input NEDT; binary
15	Input GPDT (from PEND); binary
16	Input GEDT; binary
17	Intermediate (Scratch) BCD EDT*
(BCD-to-binary mode)	
4	Output EDT; binary
5	Standard card input
6	Standard printed output
13	Input EDT; BCD format

(Note that the stand-alone nature of the BCD-to-binary mode of execution allows the apparently conflicting designation of logical unit 13.)

2.8 Variable Core Size Requirement for the SAM-X Program

The user has the option of easily varying the size of blank common in SAM-X. This enables the processing of elements with inordinate memory requirements, such as iron.

The size of blank common is specified in the MAIN program (SAMX) as follows:

```
COMMON LENTAB,TAB(20000)
   .
   .
   .
LENTAB=20000
```

In order to respecify, MAIN should be recompiled with the above 2 cards altered appropriately. For example, for iron, MAT 4180,

---

* When a CDC machine is used for binary-to-BCD conversion, this intermediate BCD EDT will contain ampersands in positive exponents of E format data. These are incompatible with IBM, and are replaced by blanks on the output BCD EDT (logical unit 4).

MOD.2 (DNA), 40,000 is used.

The variable LENTAB specifies the size of NUTRON (OVER10) only. In PEND (OVER20) and WEED (OVER30) the size of the TAB array is specified through the variables NP and NW, respectively, which are set to 20000 in the official version of the code. These variables are set in MAIN and are conveyed via labeled common PEW.

SECTION 3 - PROGRAM SAM-F

3.1 General Description of the SAM-F Program

SAM-F is a FORTRAN program, which calculates, by the forward Monte Carlo method, the time-dependent transport of neutrons or gamma rays through matter. It is a code with an overlay structure; consisting of a small driver (main overlay) and five primary overlays. These primary overlays and the functions which they perform are as follows:

> Primary Overlay 1 (AGEOM) processes the geometry input data.
>
> Primary Overlay 2 (ADATA) processes cross section and all other input data.
>
> Primary Overlay 3 (ASORTT) presorts neutron interaction and secondary gamma ray production data (secondary problems only).
>
> Primary Overlay 4 (AMONTE) performs the Monte Carlo transport calculations.
>
> Primary Overlay 5 (AMOUT) edits the results.

Basically, the program requires as input a geometry specification, the elemental composition of each region, and a specification of the location and time-energy-angular distribution of the radiation source. The program selects individual primary source particles either internally from a given source distribution or from a previously generated externaly source tape. Secondary source particles are generated internally from an external "interaction tape" (see below), usually produced by a precursor primary particle calculation.

The program then tracks the particles through a series of interactions within the geometry until such time as the particle history is terminated. The tracking of a particle can be terminated for any of the following reasons:

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1. The energy of the particle after an interaction falls below a specified "cutoff energy."
2. The elapsed time spent by the particle traversing the geometry exceeds a specified "cutoff time."
3. The particle escapes from the geometry (crosses an external boundary).
4. The particle is "killed." (This procedure will be explained in Section 3.2.10 which deals with the importance sampling techniques employed in the program.)

For each user-designated scoring region, traversed by a given particle, the code computes the number flux per second per electron-volt(ev) in energy and time bins. The flux contribution for a given particle is defined as its expected total path length* contribution in a region divided by the volume of the region. Individual particle flux contributions are accumulated so that the end result of the tracking process is the total flux in each region in a specified group of energy and time bins. (At the user's option the problem can be made time independent.) The code has the additional capability of being able to compute fluxes at specified points within the geometry. The technique incorporated into SAM-F employs a procedure which not only provides a bounded variance of all results, but a bounded esti-

---

* The "expected total path length" of a particle entering a region of length S, and total cross section μ is:

$$\int_0^S e^{-\mu s}\, ds = \frac{1-e^{-\mu S}}{\mu}$$

$$\rightarrow S \text{ (for small } \mu S)$$

mator as well.* This represents a major advance in the state-of-the-art of Monte Carlo calculations and is described, in more detail, below.

The above description of the SAM-F program is, of course, a very simplified view of the computational procedure. The following sections provide detailed descriptions of each part of the computation.

3.2 Detailed Descriptions of the SAM-F Program

In this section detailed (though, in general, nonmathematical) descriptions of the SAM-F code are presented. These descriptions are sufficiently complete so that the general user may then proceed to Section 3.4, which contains the descriptions of the input and output. However, those desiring more background knowledge of SAM-F, as well as some mathematical analysis, may wish to read Section 3.3 also.

3.2.1 Mathematical Model of the Configuration-Combinatorial Geometry

In order to perform computer studies concerning a complex three-dimensional object one must first be able to prepare a mathematical model of the object, and its environment. The Combinatorial Geometry technique, used by SAM-F, has been developed to permit a model to be produced which is both accurate and suitable for ray tracing. (Nuclear radiation analysis by Monte Carlo involves the tracing of rays through geometrical models.)

In effect, the geometric description subdivides the problem space into unique regions. This is achieved through the use of

---

*That is, infinities ("poles", caused by the usual inverse-square estimations to a point detector, are completely elminated.

ten specific geometric bodies (interiors of closed convex surfaces) and the orderly identification of the combination of those bodies which define a region (space volume). The bodies, which will be discussed further below (Section 3.2.1.2), are as follows:

1. Rectangular Parallelepiped
2. Box
3. Sphere
4. Right Circular Cylinder
5. Right Elliptical Cylinder
6. Truncated Right Angle Cone
7. Ellipsoid of Revolution
8. Right Angle Wedge
9. Arbitrary Convex Polyhedron of four, five or six sides (each side having three or four vertices).
10. Truncated Elliptical Cone.

Except for rectangular parallelepipeds, all bodies may be arbitrarily oriented with respect to the x, y, z coordinate axes used to determine the space. (The sides of a rectangular parallelepiped must be parallel to the coordinate axes.)

3.2.1.1 Re[illegible]on Description Technique

The basic technique for the description of the geometry consists of defining the location and shape of the various physical regions (wall, equipment, etc.) in terms of the intersections and unions of the volumes contained in a set of simple bodies. A special operator notation involving the symbols (+), (-), and (OR) is used to describe the intersections and unions. These symbols are used by the program to construct tables used in the raytracing portion of the problem.

If a body appears in a region description with a (+) operator, it means that the region being described is wholly contained in the body.

If a body appears in a region description with a (-) operator, it means that the region being described is wholly outside the body.

The (OR) operator is used to form regions as unions of subregions, where each subregion is defined in terms of one or more bodies, using (+) or (-) as described above. Then a point is in the region if it is in any subregion.

The technique of describing a physical region is best illustrated by an example. Consider an object composed of a sphere into which is inserted a cylinder. This is shown in cross section in Figure 3.1(a).

To describe the object, we take a spherical body penetrated by a cylindrical body (Figure 3.1(b)). Each body is numbered. Consider the sphere as body No. 1 and cylinder as body No. 2. If the materials in the sphere and cylinder are the same, then they can be considered as one physical region, say region A (figure 3.1(c)).

The description of region A would be:

A = (OR 1) (OR 2).

This means that a point is in region A if it is either inside the subregion defined by body 1 alone or the subregion defined by body 2 alone.

If different materials are used in the sphere and cylinder, then the sphere with a cylindrical hole in it would be given a different region identifier (say B) from that of the cylinder (C).

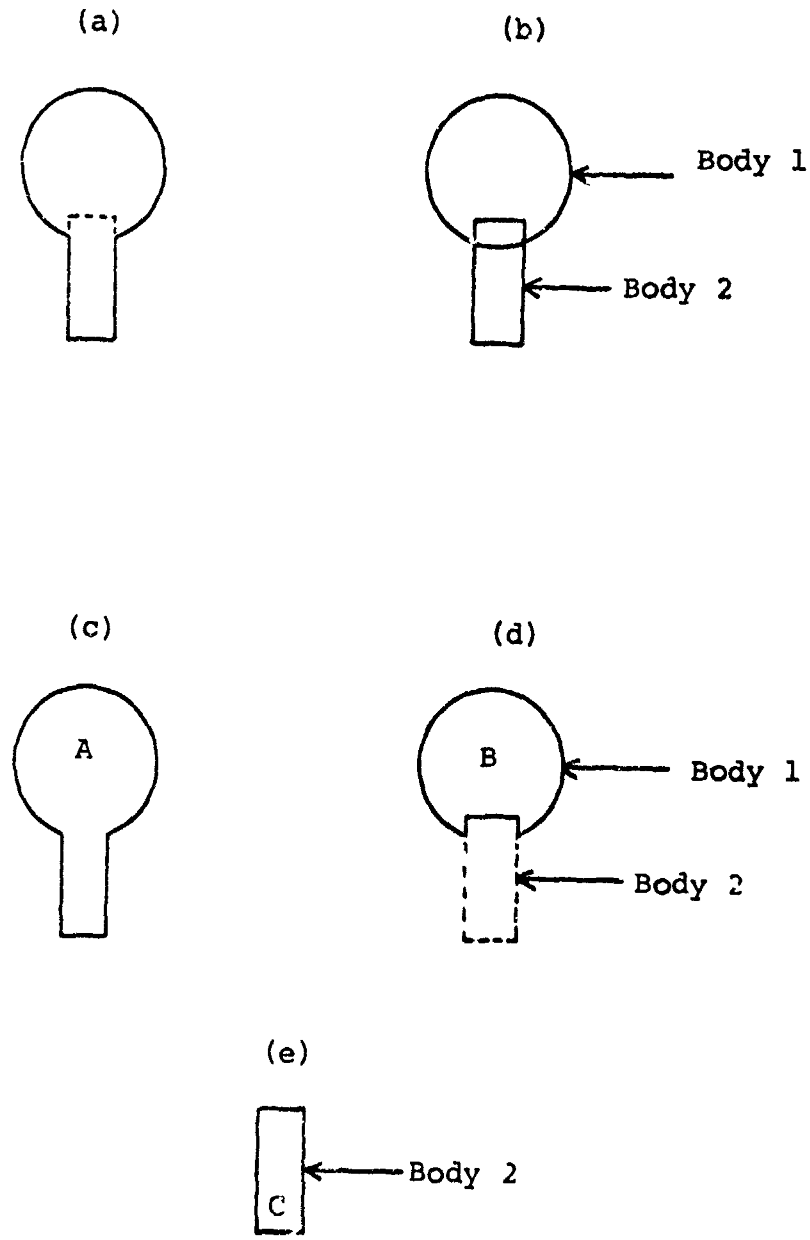


Fig. 3.. - Regions Produced by Intersections and Unions of Sphere and Cylinder

The description of region B would be (Figure 3.1(d)):

$$B = (+1)(-2).$$

This means that points in region B are all those points inside body 1 which are not inside body 2.

The description of region C is simple (Figure 3.1(e)):

$$C = (+2).$$

That is, all points in region C lie inside body 2.

This technique, of course, can be applied to combinations of more than two bodies and such region descriptions could conceivably contain a long string of (+), (-) and (OR) operators. The important thing to remember is that every spatial point in the geometry must be located in one and only one region. Further examples are given in Section 3.2.1.3.

The user of the program will specify the geometry by establishing two tables. The first table will describe the type and location of the set of bodies used in the geometrical description. The second table will identify the physical region in terms of these bodies. The computer program processes these tables to put the data in the form required for ray tracing. All of the space must be divided into regions, and, as noted above, no point may be in more than one region.

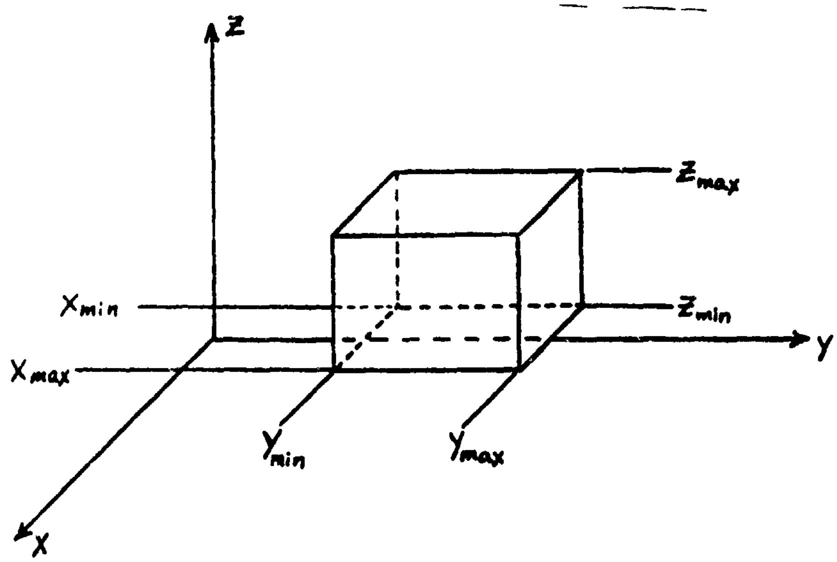
3.2.1.2 Description of Input Parameters

The information required to specify each type of body is as follows

1. Rectangular Parallelepiped (RPP)

These bodies must have bounding surfaces parallel to the coordinate axes. Tracking in an RPP is considerably faster than tracking in a box (see next body).

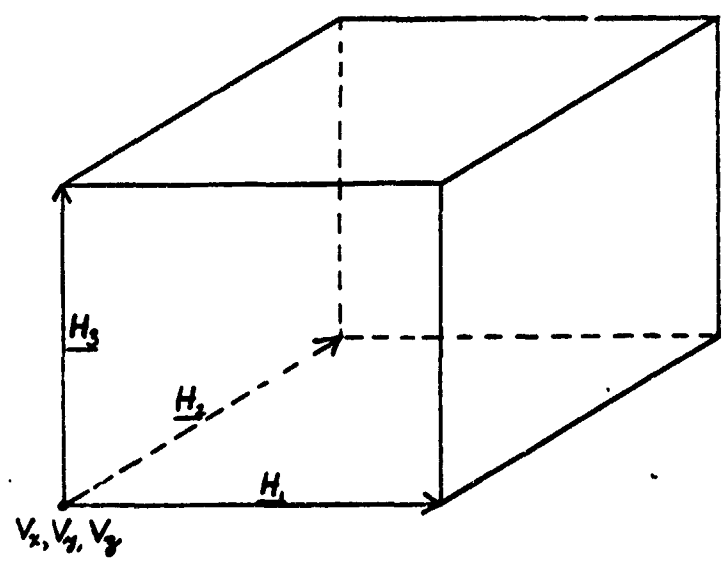
Specify the maximum and minimum values of the x, y, and z coordinates which bound the parallelepiped.



2. Box (BOX)

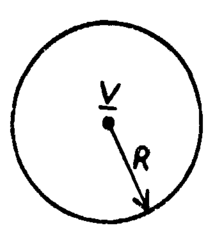
Unlike a rectangular parallelepiped the surfaces of a box need not be parallel to the coordinate axes. However, tracking in a box is slower. A box should be used only when use of a rectangular parallelepiped is not possible.

Specify the vertex $\underline{V}$ at one of the corners by giving its (x,y,z) coordinates. Specify a set of three mutually perpendicular vectors, $\underline{H}_i$, representing the height, width, and length of the box, respectively.



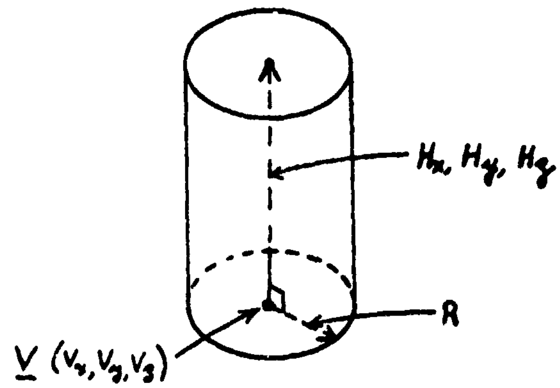
3. Sphere (SPH)

Specify the vertex $\underline{V}$ at the center and the scalar, R, denoting the radius.



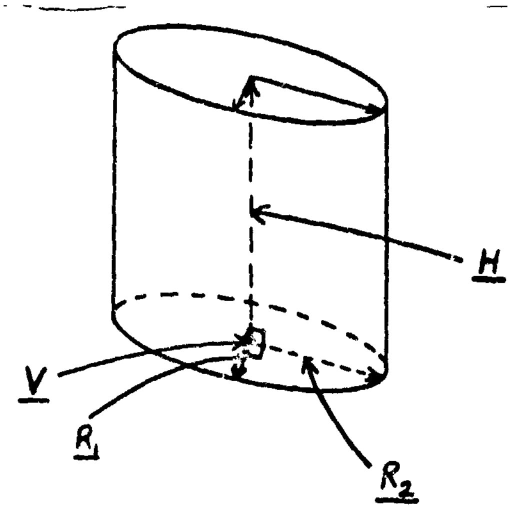
4. Right Circular Cylinder (RCC)

Specify the vertex $\underline{V}$ at the center of one base, a height vector, $\underline{H}$, expressed in terms of its x, y, and z components, and a scalar, R, denoting the base radius.



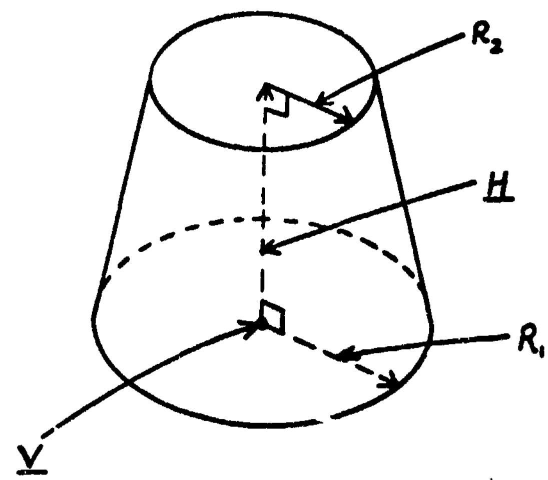
5. Right Elliptical Cylinder (REC)

Specify coordinates, $\underline{V}$, of the center of the base ellipse, a height vector, $\underline{H}$, and two vectors, $\underline{R_1}$ and $\underline{R_2}$, in the plane of the base defining the major and minor axes.



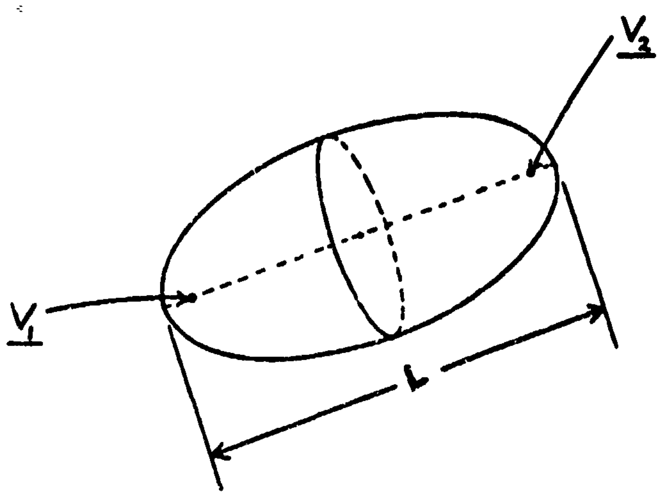
6. Truncated Right Angle Cone (TRC)

Specify a vertex $\underline{V}$ at the center of the lower base, the height vector, $\underline{H}$, expressed in terms of its x, y, z components, and two scalars, R_1 and R_2, denoting the radii of the lower and upper bases.



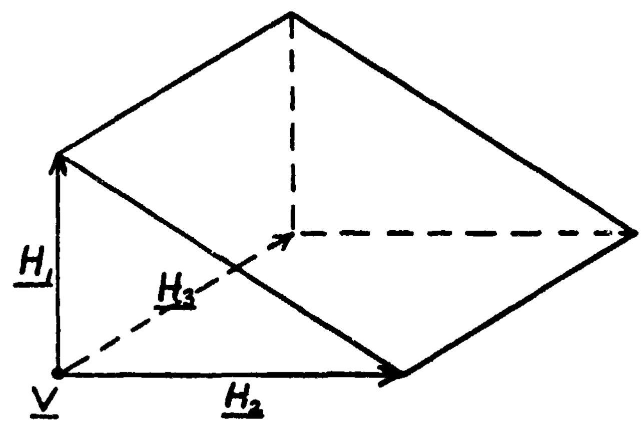
7. Ellipsoid (ELL)

Specify two vertices, $\underline{V_i}$, denoting the coordinates of the foci and a scalar, L, denoting the length of the major axis.



8. Right Angle Wedge (RAW or WED)*

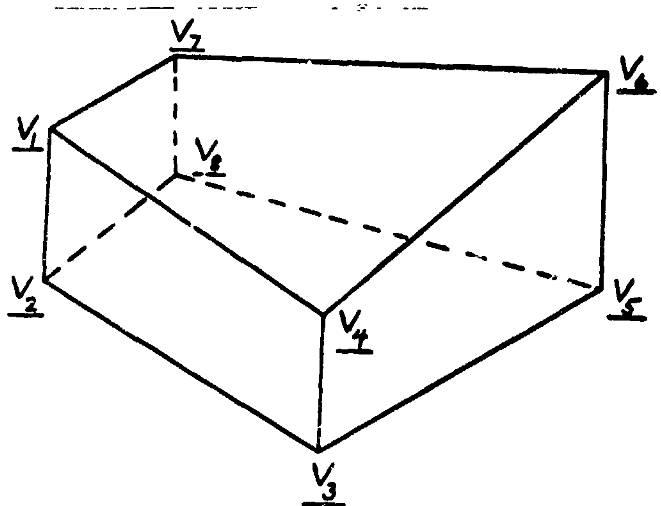
Same input as for the boxes. However, $\underline{H}_1$ and $\underline{H}_2$ describe the two legs of the right triangle of the wedge.



* Both the "RAW" and "WED" designations are acceptable as specification of the right angle wedge.

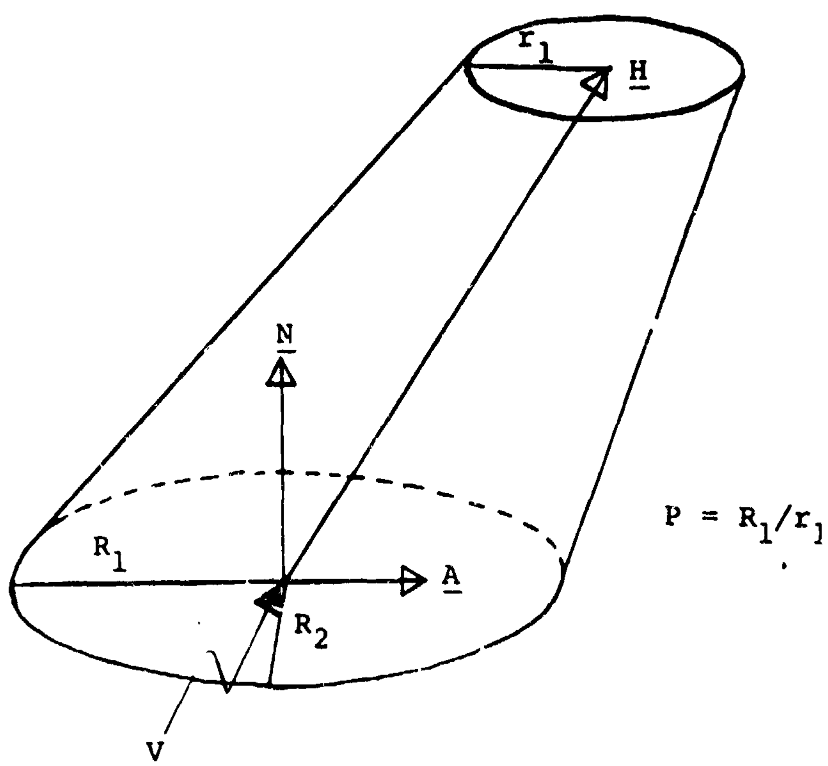
9. Arbitrary Polyhedron (ARB)

Assign an ordinal number (1 to 8) to each vertex, $\underline{V}$. For each vertex, give the x, y, z coordinates. For each side of the figure list the ordinal vertex numbers. The required ordering sequence of the vertices and the sides is given in the input section of the manual, Section 3.4.1.



10. Truncated Elliptical Cone (TEC)

Specify the coordinates of the vertex **V** at the center of the larger ellipse; the x, y, and z components of height vector **H**; the components of normal vector, **N**, directed inward at **V**; the components of direction vector, **A**, along major axis; the semi-major and semi-minor axes of larger ellipse, R_1 and R_2, respectively; the ratio, P, of the larger to the smaller ellipse axis. Note that direction vectors **N** and **A** are normalized internally (after input printout).



3.2.1.3 Examples of Region Descriptions

Some representative geometries and their input descriptions are shown below.

Example 1 - Two Spheres Within an RPP (See Figure 3.2)

The body input table is shown below.

TABLE I - BODY INPUT DESCRIPTION

Body	Type of Data Required
1	List the six bounding coordinate values (x_{min}, x_{max}, y_{min}, y_{max}, z_{min}, z_{max})
2	List the vertex and radius of sphere 2
3	List the vertex and radius of sphere 3

One possible region input table is shown below.

TABLE II - REGION DESCRIPTION

Region	Input
A	+1 -2 -3 (Region A is composed of all points interior to RPP No. 1 and exterior to spheres 2 and 3)
B	+3 -2 (Region B is composed of all points interior to sphere 3 and exterior to sphere 2)
C	+2 +3 (Region C is composed of all points which are in sphere 2 and are also in sphere 3)
D	+2 -3 (Region D is composed of all points interior to sphere 2 and exterior to sphere 3)
E	OR 2 OR 3 (If desired, one region, the total of regions B , C and D , can be defined as region E)

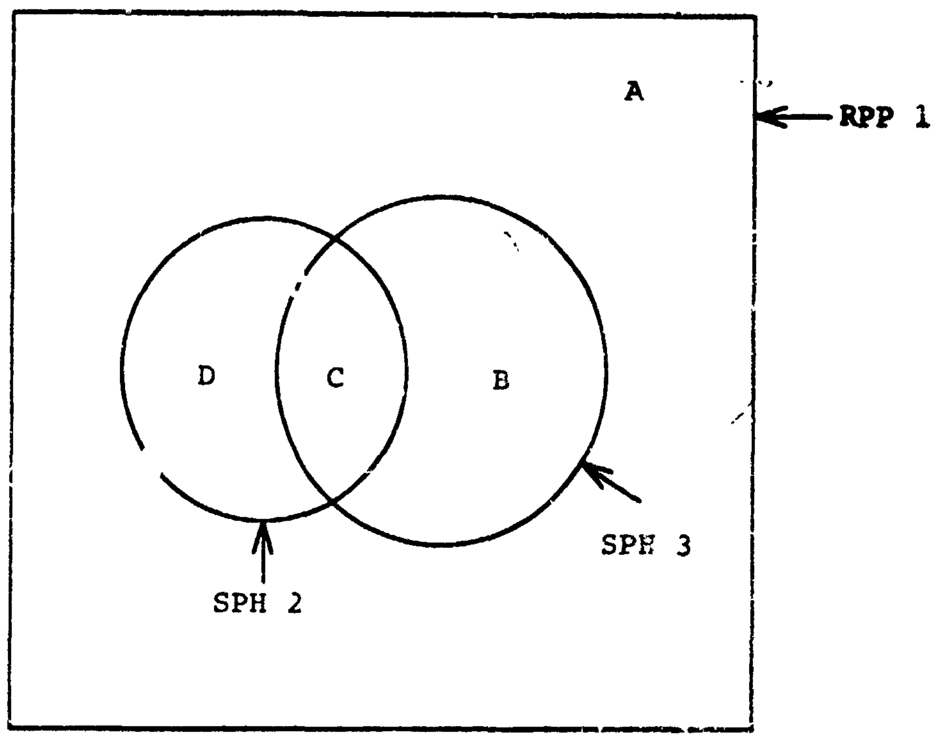


Fig. 3.2 - Regions Produced by Intersections and Unions of Two Spheres

Example 2 - Cylinder Divided into Two Regions by a Box and with a Sphere at One End (See Figure 3.3)

TABLE I - BODY INPUT DESCRIPTION

Body	Type of Data Required
1	List the six bounding coordinates of the RPP
2	List the vertex, radius, and height vector of cylinder
3	List center and radius of sphere
4	List coordinates of one corner and components of three vectors representing sides of box.

The region input is as follows.

TABLE II - REGION DESCRIPTION

Region	Input
A	+1 -2 -3 (All points interior to the RPP and exterior to the cylinder and sphere. Note that region A includes all of the space contained inside body 4, except that portion inside cylinder 2. This space can be assigned a special region number, if desired. If, as in this example, it is not desired, it is not necessary.)
B	+2 -4 (All points interior to the cylinder, and outside the box.)
C	+3 -2 (All points interior to the sphere and external to the cylinder.)
D	+2 +4 (All points interior to the cylinder and also inside the box.)

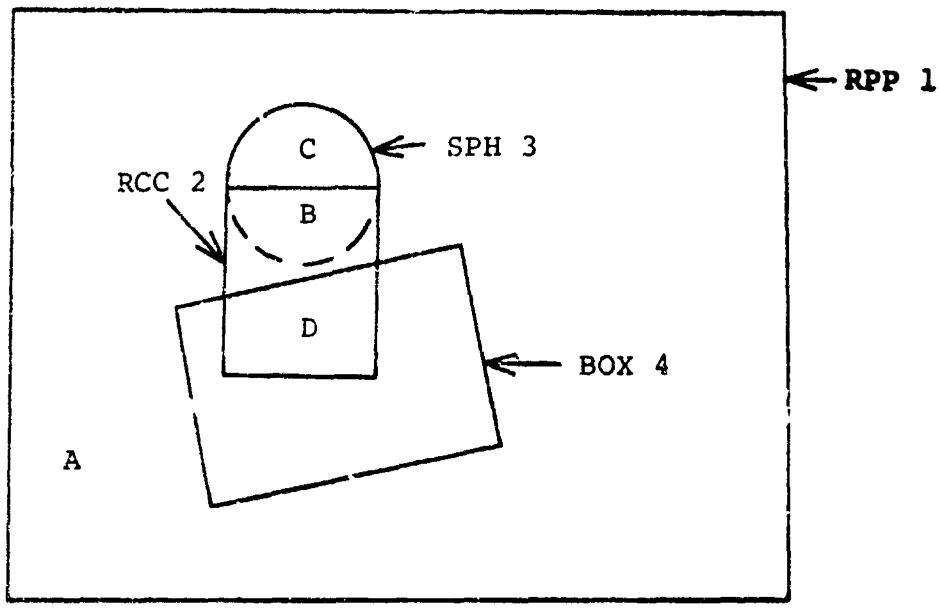


Fig. 3.3 · Regions Produced by Intersections and Unions of Sphere, Circular Cylinder, and Box

Example 3 - Multiple Region Capability - Cylinder Containing Two Spheres, All Inside an RPP (See Figure 3.4a)

TABLE I - BODY INPUT DESCRIPTION

Body	Type of Data Required
1	RPP input
2	Cylinder input
3	Sphere input
4	Sphere input

TABLE II - REGION DESCRIPTION

Region	Input
A	+1 -2
B	OR 3 OR 4 (All points interior to Body 3 or Body 4)
C	+2 -3 -4 (All points in the cylinder but not in the spheres.)

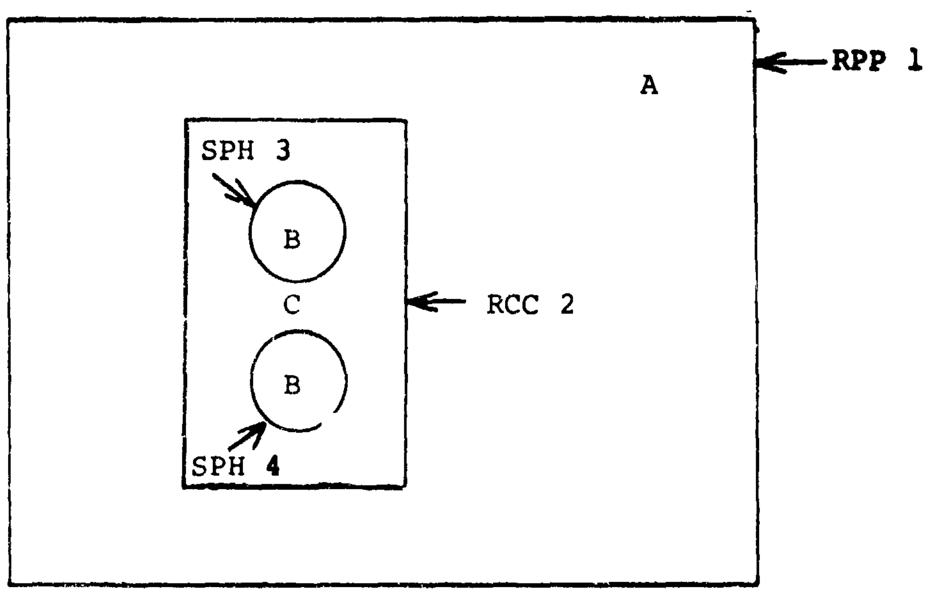


Figure 3.4a - Example of Physical Region Produced from Unconnected Regions Using "OR" Statement.

Example 4 - More Complicated Use of the (OR) Statement

(See Figure 3.4b)

As a more complicated example of the use of the (OR) operator, consider the system in Fig. 3.4b consisting of the shaded region, A, and the unshaded region, B. These regions can be described by the two boxes, BOX1 and BOX3, and the sphere, SPH2.

TABLE I - BODY INPUT DESCRIPTION

Body	Type of Data Require
1	Box input
2	Sphere input
3	Box input

TABLE II - REGION DESCRIPTION

Region	Input
A	+1 +2
B	OR +3-1 OR +3-2

Note that the OR operator refers to all following body numbers until the next OR operator is reached. Hence the implied description of region B is OR(+3-1) OR(+3-2)

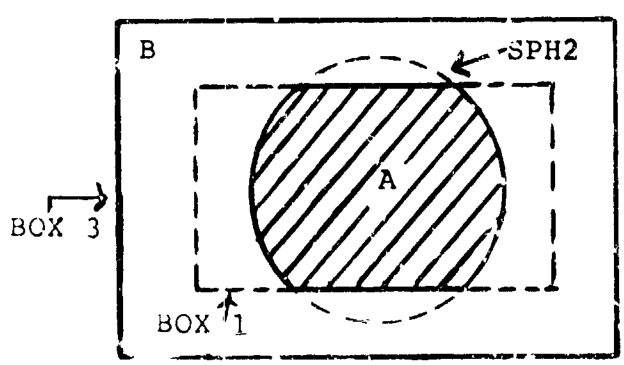


Fig. 3.4b - More Complicated example of the OR operator.

Example 5 - Combinatorial Geometry Example Employing all Allowed Body Types*

The final example, Shown in Figure 3.4c, may also be used as a check of the entire Combinatorial Geometry package. (A complete card image description is given as Appendix P).

TABLE I - BODY INPUT DESCRIPTION

BODY		TYPE OF DATA REQUIRED
1	RPP	RPP input
2	BOX	box input
3	TRC	truncated right cone input
4	REC	right elliptical cylinder input
5	ARB	ARB input
6	RAW	wedge input
7	RCC	right circular cylinder input
8	ELL	ellipsoid input
9	SPH	sphere input
10	TEC	TEC input

* Based upon a suggestion of D. DeLapp, McDonnell-Douglas Astronautics Corporation.

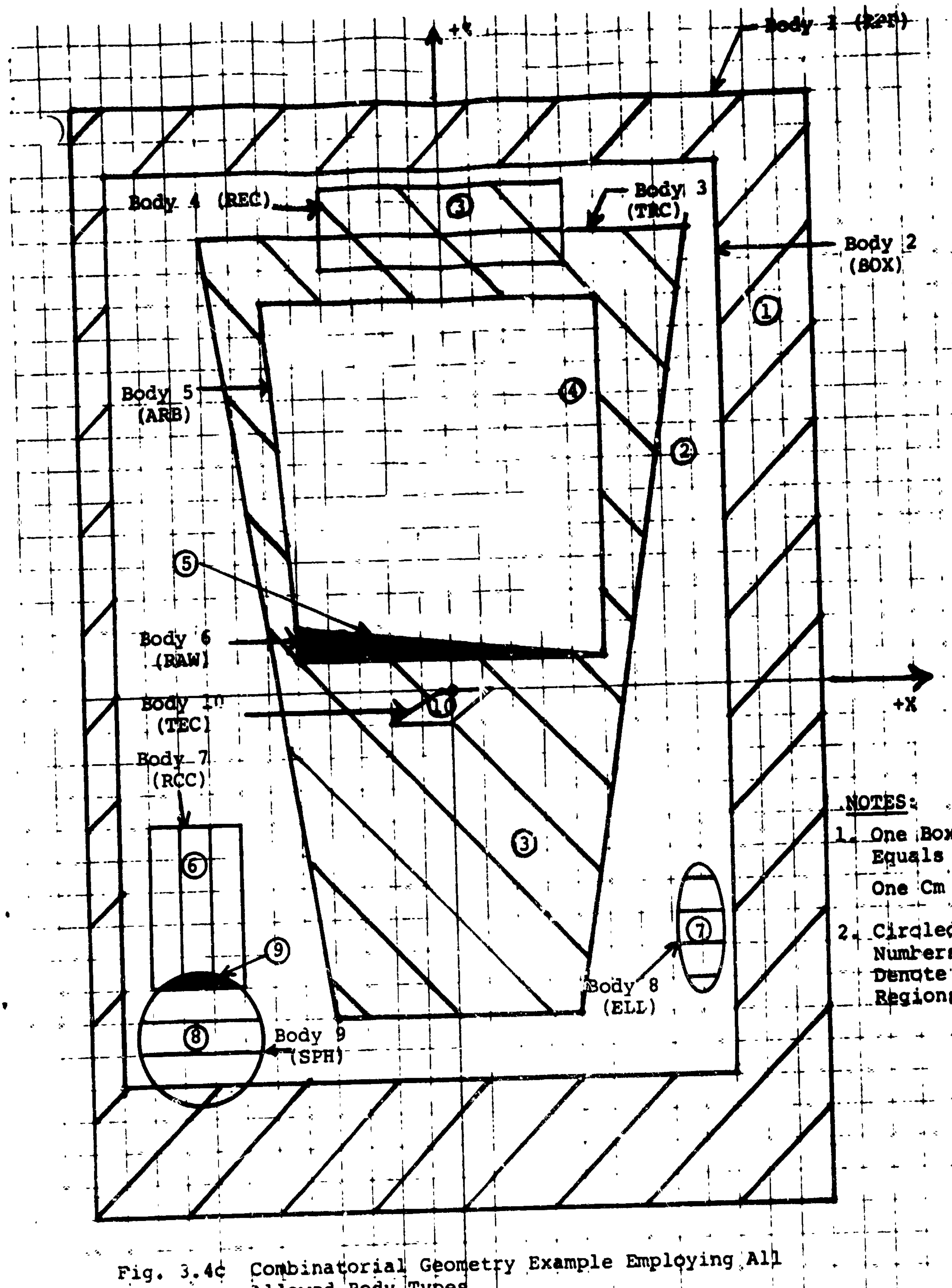


Fig. 3.4c Combinatorial Geometry Example Employing All Allowed Body Types

TABLE II - REGION DESCRIPTION

(region numbers are circled on Figure 3.4c for clarity)

REGION	INPUT
1	+1 -2
2*	+2 -3 -4 -5 -6
3	OR +3 -5 -6 -10 OR +4
4**	+5 -6 -7
5	+6
6	+7 -8 -9
7	+9 -8
8	+9 -8
9	+8 +9
10	+10

* Bodies 5 and 6 project outside body 3 in the X-Y plane (see Appendix P)

** Bodies 5 and 6 buttress each other. The negation of body 6 here eliminates possibility of machine round off error. Negation might not be necessary on CDC machines.

3.2.1.4 Automatic Checking of Combinatorial Geometry Input

Although Combinatorial Geometry is relatively simple to employ, user-specified input errors often occur for configurations involving many bodies and regions. Some of these input mistakes are difficult to spot and could, in some cases, cause the computation to terminate in the midst of execution, and could also, in other cases, lead to completely erroneous computational results.

Hence, geometry checking routines have been added to the Combinatorial Geometry package. These routines may be employed by the user, as an option, to locate and flag errors in the geometric specification.

Five different types of geometry checking are employed. Each of these is described briefly, below:

1) Errors in Body Data

Simple errors in the descriptions of the individual bodies, themselves, are located and flagged. These body checks are as follows (refer to Section 3.2.1.2):

RPP - $X_{max}>X_{min}$, $Y_{max}>Y_{min}$, $Z_{max}>Z_{min}$

BOX - Check orthogonality of three vectors describing the body

SPH - $R>0$

RCC - $R>0$

REC - Same as BOX

TRC - $R_1, R_2>0$

ELL - L > distance between foci

RAW - Same as BOX

ARB - 0,3 or 4 edges found for each face
All points defining a given face are co-planar
Body is convex

TEC - $N \perp A$
$N \cdot H>0$
$R_1, R_2>0$

2) Simple Errors in Region Descriptions

The geometry checker examines the region descriptions and determines if references are made to non-existent bodies. It also verifies that all bodies are referred to positively at least once and that all bodies, except the surrounding escape region, are referred to negatively at least once. A complete table of all bodies and the regions in which they are referenced is provided. Positive and negative references are distinguished.

3) Visual Displays

As a visual aid to the user, the checking routines can provide printer plots of arbitrary two dimensional cuts through the geometry. Scales can be stretched or compacted in one of the two dimensions. Default or user-supplied character sets may be used for the printer plot displays.

4) Checks of Suspected Points in Space

The code will locate the region corresponding to any number of arbitrary suspected points in space supplied by the user. The code will flag for the user any point which lies in an undefined or multiply-defined region of space (see following item).

5) Undefined and Multiply-Defined Regions

Perhaps the most significant aspect of the geometry checking is the flagging of undefined and multiply-defined regions of space - a common (and difficult to locate) type of Combinatorial Geometry input error.

As a very simple example, consider figure 3.5a which shows a subsection of a more complex geometry, wherein Box 1 and Box 2 specify two regions, A and B, as shown. In this correct description, all of space bounded by the two boxes is singly defined.

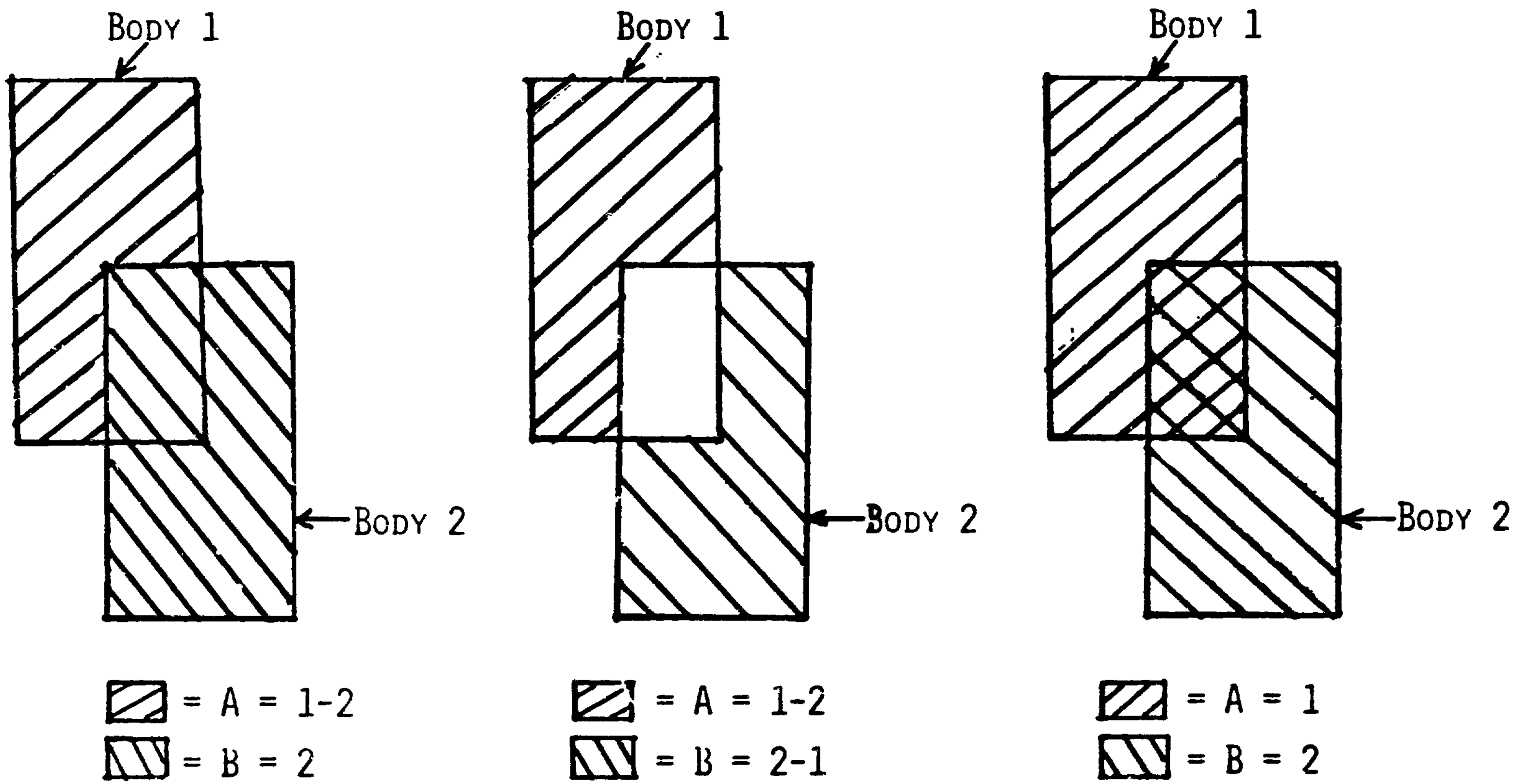


FIG. 3.5A FIG. 3.5B FIG. 3.5C

FIG. 3.5 UNDEFINED AND MULTIPLY-DEFINED REGIONS

One possible type of input error is shown in figure 3.5b wherein the overlap area remains undefined. Another type of error is shown in figure 3.5c wherein the overlap area has been doubly-defined.

At the present time, the checking routines are not yet complete. Undefined and multiply-defined regions are currently located for all situations involving the intersection of two bodies, both of which are composed entirely of planar surfaces. Also, these errors are found for some situations involving both planar and non-planar bodies. The generalized two- or three-body intersection problem, involving all types of bodies will be available in the Revision D package. Such coding is currently under way.

In the meantime, as an aid to the user, the checking code does flag all possible intersections (or buttressing) of two or three body sets. One can use this information to check partially for possible region definition errors.

3.2.2 Cross Sections and Region Compositions

Generally, the user will have at his disposal an Element Data Tape (EDT) which contains, for every isotope in the problem, a set of energy-dependent interaction cross sections. Two cross section data tapes, one for neutron problems, the other for gamma ray problems are available. (The formats of the neutron and gamma ray EDTs are given in Appendices A and B, respectively.)

The user must then specify each of the material compositions appearing in the problem. A composition must first be identified by a composition number and by the number of nuclides it contains. Next, the composition is defined in terms of atomic concentrations (in units of 10^{24} atoms/cm^3) of each nuclide in the composition. These may be calculated from the expression:

$$\frac{\rho N_o}{A} \times 10^{-24}$$

where N_o = Avogadro's number = 0.6023×10^{24} (atoms/mole)

A = atomic weight (gms/mole)

ρ = mass density of nuclide in the composition (gm/cm^3)

This input is processed in conjunction with the EDT by the BAND routine, which generates an Organized Data Tape (ODT). The ODT contains all concentrations, cross sections, and scattering data for each specified nuclide. During the tracking process this information is used to determine:

1. The probability that a particle has an interaction in a region of given composition,
2. The element with which the particle interacts,
3. The type of interaction (absorption, elastic scattering, etc.) occurring,
4. The energy and direction of the particle after a nonabsorption interaction.

The organization of the ODT is given in Appendix C.

If the user is running a secondary gamma ray problem, using as input an interaction tape produced by the primary neutron problem (see Section 3.2.16), a gamma ray production data tape must also be available. Those data are used to convert neutron interaction events into sources of the secondary gamma rays. The format of the gamma ray production data tape is given in Appendix D.

3.2.3 Cross Section Bands, Output Energy Supergroups and Superbins

Often, the user is faced with a situation involving a very complex geometry containing many different materials and distinct nuclides. Under these conditions, particularly if nuclides exhibiting many important resonances are involved, much data may be required to describe adequately the nuclear interaction and scattering processes. Hence, the amount of computer storage required to describe the entire problem, may exceed that which is available to the user.

This situation is treated by using, as options, the cross section band, supergroup, and superbin capabilities of the code. These options are now described. Further information is provided in Section 3.6.

3.2.3.1 Cross Section Bands

The overall energy range of the problem is subdivided into smaller energy ranges, and "bands" of cross section data are generated, each containing the reduced amount of cross section data appropriate to that range. These bands can be shuttled into and out of core memory, one at a time, during the Monte Carlo stage of the calculations (see below). Thus this option reduces the amount of cross section data required by the code at any one time.

3.2.3.2 Supergroups

The supergroup option divides the entire output (i.e., final score) energy range into smaller ranges. In the Monte Carlo calculations scores are accumulated in memory in only one output energy range at a time.

3.2.3.3 Superbins

The two energy meshes (bands and output supergroups) do not necessarily coincide. SAM-F combines the two meshes into a set of "superbins". As shown in Section 3.3.2 (discussion of AMONTE routine) the code performs the Monte Carlo in one superbin at a time, starting with the highest energy bin and working downwards. If a tracked particle degrades to a lower energy superbin, its parameters are stored on a disk file, and its tracking is resumed later only after all higher energy superbins have been completed.

By use of the superbin option, SAM-F is capable of treating the exceedingly complex situations referred to above.

3.2.3.4 Energy Mesh Specification

The energy boundaries for the cross section bands are automatically determined by the code in a manner which keeps the amount of cross section data in each band nearly constant. (If desired, the user may override the automatic banding option and specify the band limits himself.)

The supergroup structure is defined by the user at the same time that he inputs to the code the desired energy bin structure for the final output scores. This is done by placing a minus sign before those output energies he wishes to designate as supergroup limits. (If this option is not desired, only the upper and lower energy bin limits require minus signs. This instructs the code to treat all energies as part of a single supergroup.)

3.2.4 Source Specification

The specification of the initial particle source provides the user with several options. These options are described briefly below.

3.2.4.1 Internally Generated Source

Spatial Distribution

Sources may be generated in any number of regions, but the regions must be single bodies and restricted to SPH, RCC, BOX and RPP.* For each source region the 'total power' (particle density x volume) must be given. The user has the option of normalizing the problem to a unit source or to the total input power density.

Note that if the user-specified number of source regions is not greater than zero, this is a flag to the program to use an external source tape (one which has been generated from a previous problem or by some other means) (see Sections 3.2.4.2 and 3.2.4.3).

---

* If the need arises, this limitation could be readily altered.

Angular Distribution

Sources may be either isotropic or monodirectional but the same angular distribution must be used in all source regions.* (It should be noted, however, that a source may be generated in a finite cone by specifying an isotropic distribution and using exceedingly high, (e.g., 10^{10}) angular weights to kill particles which are generated outside the desired cone.)** At the present time, the source must be isotropic if uncollided flux-at-a-point estimates (Section 3.2.8) are to be made.

Energy Distribution

The code has built into it the Cranberg fission neutron spectrum. If this option is selected, no energy spectrum input is required. If an arbitrary spectrum is desired, the input must contain the desired energy mesh and the integrated source above each energy point (i.e., a table of E vs $\int_E^{E_{max}} S(E)dE$ is required). Monoenergetic sources may also be specified.

Time Distribution (Time-dependent problems only)

If a time-dependent problem is to be run, the user must supply a table of time values and the integrated source up to each time (i.e., t vs $\int_0^t S(t)dt$). As an option, all radiation may be emitted at a user-specified single value of time.

3.2.4.2 External Source

The user may supply an externally generated source tape. Each source particle must be described by 14 parameters in the following order:

---

* Angular biasing of an isotropic source is permitted, however.

** See Section 3.2.10 for discussion of angular weights.

3 Cartesian Coordinates (cm.) (floating point)

3 direction cosines (floating point)

1 energy (ev) (floating point)

1 geometric region number (integer)

1 time (sec.) (floating point)

1 unused parameter; enter a zero here.

1 weight (floating point)

1 history number (integer)

1 extra carry along weight; enter a 1 here (floating point)

1 particle type index; enter a 1 here (integer)

These data must have been written previously, by a separate program, on a file designated as tape 15, as a series of binary records for 35 particles at a time; i.e., (14 parameters per particle) x (35 particles/record) = 490 parameters per record.

Given the array A(14,35) the proper output statement is*

WRITE(15) ((A(I,J),I=1,14),J=1,35).

3.2.4.3 Source from Previously Generated Interaction Tape

Using a neutron interaction tape (see Section 3.2.1), and gamma ray production data supplied by SAM-X, SAM-F can generate, internally, sources of secondary gamma radiation. Note that the interaction tape was generated by a previous SAM-F calculation and has a form similar to that of the external source tape of Section 3.2.4.2. (See Table 3.2, below, for a complete description.)

---

* Experienced programmers prefer, of course, WRITE(15) A which is considerably faster.

3.2.5 Output Energy Mesh

During tracking, the code stores fluxes in each region in a set of energy output bins specified by the user. The number (≤ 100) and width of these bins are arbitrary. The bin limits must be given consecutively in the input, starting with the highest energy. The upper and lower bin limits for all supergroups must be preceded by minus signs as explained in Section 3.2.3. Care should be taken to insure that the upper energy bin limit is equal to or greater than the highest source energy to be generated in the problem. A cutoff energy is also specified, which instructs the code to cease tracking any particle which degrades below this energy.* The user should be certain that the lowest energy bin limit is lower than the cutoff energy. In essence, there must be a bin available to store every possible energy in the problem.

(In order to simplify matters for the user, Appendix E gives the hierarchy table for all input energy limits and tables.)

3.2.6 Time Dependence

SAM-F enables the user to compute particle fluxes as a function of time as well as energy and position. The user selects any desired time bin structure for the problem and enters the bin limits in consecutive order on the input forms, starting with the highest bin. Output fluxes will be given in this bin structure in the edit.

---

* However, see Section 3.2.11, for discussion of the thermal neutron option.

The longest time, used in specifying the time bins, will be used by the code as the time-cutoff parameter. During the tracking process the code computes the flight time of a particle between collision points from its velocity (or energy). All nuclear interactions are assumed to occur instantaneously. By accumulating the flight times for each particle, the code is capable of storing particle fluxes in the proper output time bins.

3.2.7 Scoring Regions

A scoring region is one in which a flux contribution is computed for each particle which passes through it. In a nonscoring region no such computation is made, so that the output edit provides fluxes only in those regions designated in the input as scoring regions.

In some problems it is desired to know the flux in every region separately, in which case each region in the problem would be defined as a scoring region with a different number. In some problems, however, two or more regions may be completely symmetric with respect to the source, in which case the fluxes in these symmetric regions could be combined without any loss of information, and in fact, an improvement in the accuracy will be obtained. Each of these regions then would be designated by the same scoring region number. In still other problems it may be unnecessary to know the fluxes in certain regions. These should then be given scoring region number zero, which tabs them as nonscoring.

Since fluxes are stored and printed out for scoring regions only, it is possible to reduce both the size of the edit and the core storage requirements by reducing the number of different scoring regions. It should be remembered, however, that once a problem is run it is impossible to recapture any flux information in nonscoring regions except for the flux-related collision, absorption, degradation and time-kill densities (given for each scoring and nonscoring region), integrated over all time and energy.

3.2.8 Flux-at-a-Point

In certain problems it may be desired to calculate the flux at a particular point, or points, in the geometry. Since, during the ordinary tracking process, no particle can be expected to pass through a given point, SAM-F incorporates a method of estimating flux at one or more specified points.

SAM-F performs the flux-at-a-point calculations with a new "bounded" estimator developed at MAGI. The detailed description of this estimator is reserved for Section 3.3.2.

3.2.9 Flux-in-a-Small-Volume

In certain situations the detector is finite in extent but yet too small for efficient use of the usual track length scoring procedures, (e.g., experimental configurations involving counting detectors). Providing the detector is a sphere, cylinder, or box, the user may designate such a region as a "small volume" detector and the code will estimate the flux in the detector. More than one small volume detector can be treated simultaneously.

The mathematical description of the flux-in-a-small-volume routine is reserved for Section 3.3.2.

3.2.10 Importance Sampling

General

Importance sampling or "weighting" provides the user with a powerful method of controlling the direction and/or energy of particles in the problem. The purpose of a particular problem, for example, may be to calculate the fast-neutron flux in a given region within the geometry. Under normal circumstances, the probability of a source neutron reaching that region at high energy may be quite small, requiring a vast number of source neutrons to be tracked before an adequate statistical estimate of the flux is obtained. However, with proper particle weighting the code can be made to concentrate only on those fast neutrons having the best chance of reaching the chosen region. Conversely, the code will spend little time tracking neutrons which are either traveling in the wrong direction or are at relatively low energy.

The program determines the relative importance of a particle from a parameter called the weight. The total weight (W) of a particle is, in turn, determined from a combination of three quantities called region weight (W_R), angular weight (W_Ω), and energy weight (W_E), where $W = W_R \times W_\Omega \times W_E$. Values of W_R, W_Ω, and W_E must be supplied as input. The following brief discussion should provide the user with a better insight into how these weights are actually used by the code.

A quantity F is assigned to each particle. The value of F is 1.0 for a source particle. The code calculates the probability that the particle will reach the boundary of the source region along its flight path without collision. This value is called F".

The probability that a collision takes place in the region is then 1-F". The code picks a random number and with probability 1-F" creates a collision point inside the source region at a point picked from an exponential probability distribution. The source particle history is not terminated but continues to the boundary of the region. (Note that after this source particle has been completely tracked, the code will return to this collision point, do the proper collision mechanics, and start a new particle (latent).

Suppose that the source particle is leaving region 1 where the weight is W_1 and entering region 2 where the weight is W_2. At the boundary, the ratio of weights W_1/W_2 is multiplied by F" and the particle is given a starting value of F=F" W_1/W_2 in region 2. The probability of the particle reaching the next boundary of region 2 uncollided is calculated and multiplied by F to obtain a new value of F". In region 2 a number of collision points approximately equal to F-F" will be produced. Notice that if W_2 is large compared to W_1, the probability is high that no latents will be produced since both F and F" will be small compared to one. In fact, a parameter F_z is an input to the program. If F, on entry into a new region, is lower than F_z, a random number between zero and one is picked. If the number is greater than F the history is terminated. If it is lower than F, the history is continued with F set equal to one.

Thus, by establishing weight sets properly, increased numbers of collisions can be forced to occur in important regions, and in addition, the original source particles will continue to propagate through the geometry.

Without going into detail, it can be stated that a small value of F_z minimizes the number of kills (increases problem running time). A large value maximizes the kills (decreases running time per history) but increases the variance of the answers, requiring more source particles to be run. The optimum value of F_z will generally lie in the range from 0.01 to 0.1.

In order to facilitate input preparation, the three components of the total weight will now be discussed separately.

Region Weights

A region weight (W_R) must be specified for every region in the problem. Ordinarily, these weights are set up so that they gradually decrease as a particle proceeds from the source toward a region in which the flux is desired. Weights should gradually increase in regions which are located progressively further from the "important" regions. On the input forms the user must specify all values of W_R to be used in the problem. The order in which these values are entered determines their region weight index (i.e., the first value of W_R is assigned index 1, the second value is assigned index 2, etc.). Then for each region, the weight index to be used in that region must be specified.

Angular Weights

By using angular weighting, it is possible to specify preferred directions for a particle, independent of the region location of the particle. The user first specifies the direction cosines (with respect to the coordinate axes of the problem) of

one or more aiming angles. These vectors serve as "zero directions" about which angular weights will be given. Each aiming angle is assigned an index. Next, a set of angular bins is specified between 0° and 180°, with the bin boundaries given in terms of their cosines. Thus, if one desires to specify four bins of equal angle, the cosines of 0°, 45°, 90°, 135°, and 180° should be entered. Then, one or more <u>sets</u> of angular weight values are given. For each set, a weight value (W_Ω) is specified for each angular bin. Each set is also assigned an index. Finally, for each region, the aiming angle index and the angular weight set index must be given. To illustrate how the code uses this information, assume that a given region has been assigned aiming angle #1 and angular weight set #2. A particle enters the region and the code determines that the particle is traveling at an angle ϕ with respect to aiming angle #1. The code then determines which angular bin encompasses ϕ, goes to angular weight set #2, and finds the value of W_Ω in that bin.

In general, as the particle direction (angular bin) becomes more important, the value of W_Ω assigned to that bin should decrease.

<u>Energy Weighting</u>

The use of energy weighting enables the user to instruct the code as to which particle energies are more important in a given problem. A set of energy bins is first given, where the bin boundaries are listed in decreasing order. Then, one or more

energy weight sets are specified, with each set being assigned a number. For each set an energy weight value W_E must be given for each energy bin. The energy weight set number corresponding to each region is then given. Assume, for example, that a particle of energy E is in a region which has been assigned weight set #1. The code first locates the energy bin which encompasses E, refers to weight set #1, and determines the value of W_E which was given for that bin. In establishing the energy weights, the more important energies should generally have smaller W_E values than the less important energies.

Application of Weights to Tracking

As noted earlier, the total particle weight is the product of $W_R \times W_\Omega \times W_E$. The particle weight is used to determine the number of collisions that a particle will produce given that it has a specified energy and direction in a given physical region. By an appropriate choice of aiming angle and angular weights, particles heading downward can be caused to have more collisions than particles heading upward in the same region. Thus, more computing time will be spent on the "important" downward directed particles and their descendents than on the "less important" upward directed particles.

Treatment of "Latent" Particles

If a collision does occur, the program calculates the energy and direction of the particle emerging from the collision. The collided particle is stored* in a latent storage table and will be

* If the energy of the particle emerging from collision is below the current "superbin" limit (See Sect. 3.2.3), then the particle is placed in a separate latent table (of unlimited capacity, i.e., tape or disk storage is used) for later processing.

picked up and followed as though it were a source particle at a later time. When it is started out as a real particle, it is assigned an F value equal to the ratio of the weight of the particle before collision to the weight of the particle emerging from collision. In general, these will be different due to differences in energy and direction of travel.

The program stores the information concerning latents in a table which can hold up to 100 latents. Prior to storage a test is made to see if the F of the latent exceeds the input value of F_z. If so, it is stored. If not, a Russian roulette calculation is performed, as previously discussed, and the latent is either eliminated or has its F set equal to 1.0.

If more than 100 latents are generated by a source particle, the program has a "squeeze" routine which reduces the number of latents in a statistically valid way.

Although the use of importance sampling may appear to be a rather complicated procedure, the user will generally find that after gaining a little experience with the code the process becomes relatively straightforward and easily applied. Certainly, the time spent in learning how to apply properly this technique will be well worth it in the long run, since it enables complex, deep-penetration problems to be run in a reasonable amount of machine time. Appendix F contains a discussion of the theory of importance sampling with an example of how a set of weights is established.

3.2.11 Thermal Neutron Option

The normal procedure for neutron scattering, as implemented in SAM-F, assumes the interacting nuclide to be at rest. The process thus allows for energy degradation only. The degradation process continues from birth (source energy) down to the point where the neutron energy falls below a user-specified "low energy cutoff" (ECUT). At this point the particle is killed.

The thermal neutron option is invoked by entering a "thermal energy" (ETHERM) which is slightly greater than ECUT. (Item 21 of input - see Section 3.4.1.3). When a particle degrades by scattering below ECUT, its energy is changed back to ETHERM, and normal transport continues at that energy. The "thermal group" problem is therefore solved using the single velocity approximation. The following effort is made to use effective thermal cross sections.

At input processing time, the point value cross sections at the thermal energy ETHERM are replaced by Maxwell-averaged cross sections.

For each "i-th" nuclide

$$\bar{\sigma}_i = \int_0^{\infty} \sigma_i(E) \frac{1}{T^2} e^{-E/T} dE$$

where T = ETHERM.

The integration is performed using linear interpolation on $\sigma(E)$ in the energy range of the element data tape (standard procedure for SAM-X output), an energy independent extrapolation to higher energies, and an extrapolation to zero energy in the form $\alpha + \beta E^{-\frac{1}{2}}$.

Once the thermal neutron option has been specified by the use of ETHERM (where ETHERM>ECUT), a thermal neutron diffusion approximation option can also be invoked. This is discussed in the following section.

3.2.12 Thermal Neutron Diffusion Approximation

If the thermal neutron option (Sect. 3.2.11) has been specified, an additional option is available to specify the use of a thermal neutron diffusion approximation.

As is well known, thermal scattering of neutrons in large media with small absorption, produces large numbers of collisions. In the Monte Carlo game, the exact simulation of the transport process can thus lead to prohibitively lengthy computations. Fortunately, in this case, the transport equation can often be approximated by the diffusion equation.

The implementation of the diffusion approximation in SAM-F is currently limited to a single homogeneous rectangular parallelepiped with edges parallel to the Cartesian coordinates. The parallelepiped can overlap, or partially overlap, any number of regions provided they all consist of the same material composition.

If a particle degrades to thermal energy inside the "diffusion box," the diffusion subroutine samples from internal tables and generates either an absorption event inside the box, or an escape through the sides of the box. If the event is an escape, the particle is subsequently tracked by normal transport methods in the regions outside the diffusion box.

3.2.13 Number of Histories and Statistical Groups

The user must designate the total number of source particles (histories) to be run in the problem. Although a greater number of histories will improve the accuracy of the answers, it will also increase the problem running time. The user must, therefore, strike a balance between the tolerable errors in the answers and the cost of running the problem. In complicated problems it is usually wise to run a test problem of 100 to 1000 histories to get a "feel" for whether particles are reaching the desired regions. If they are not, the fault probably lies in incorrect importance sampling and the weights should be adjusted. If the test problem appears to have run "well", then the number of histories can be increased by perhaps a factor of about 10. After some experience, the user can generally determine the correct number of histories to run in a particular problem.

In running the problem, the total number of histories is divided into aggregates called statistical groups. This is done in order to compute the variance (or standard deviation) of the fluxes. All particles (and their latents) within a group are tracked before another group is treated. Fluxes are computed and stored on tape separately for each group. The size of the statistical group is constant in a given problem and must be specified in the input. The use of about 20 statistical groups per problem generally has been found to be adequate.

3.2.14 Volume Computation

To evaluate the flux, the history-averaged track length scores in a region are divided by the volume of the region.* Provision has been made to input volumes of regions if they are known. It often happens, however, that regions described by the Combinatorial Geometry technique have such complex shapes that an analytic volume computation is not practical. To determine the volume of such regions, a routine is included to perform a ray-tracing numerical integration calculation of the volume.

A point $\overline{X}$ within the geometry is given as input. Rays are randomly fired isotropically from the point $\overline{X}$ and the volume of each region is then

$$V_i = \frac{4\pi}{3H} \sum_{k=1}^{H} (R_{2,k}{}^3 - R_{1,k}{}^3)$$

where $R_{1,k}$ and $R_{2,k}$ are the distances of the k^{th} ray to the first and last contacts with region i. "H" is the total number of rays fired.

The accuracy of the computation is thus dependent on the number of rays fired.

Provision is made for the input of pre-computed volumes where great accuracy is desired.

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* $\frac{\text{Track length (cm)}}{\text{Volume (cm}^3)} = \text{Flux (cm}^{-2})$

3.2.15 Response Functions

SAM-F provides a response function option which allows the user to transform particle fluxes, automatically, into up to 6 desired flux-dependent quantities (dose, heat deposition, etc.). Assume, for example, that the dose, D, is required in several regions. The user supplies, as input, a flux-to-dose conversion factor as a function of energy. For each region, the code multiplies the average number flux per ev in each energy bin, by the corresponding energy-dependent conversion factor.

Let $$\phi_i(\bar{E}) = \int_{\substack{\text{ith}\\ \text{energy}\\ \text{bin}}} \phi(E)\,dE \Big/ \int_{\substack{\text{ith}\\ \text{energy}\\ \text{bin}}} dE \qquad \text{(average flux in energy bin i)}$$

and $C_i(\bar{E})$ = average conversion factor in ith energy bin.

Then $D_i(\bar{E}) = \phi_i(\bar{E}) \times C_i(\bar{E})$ and

$$\text{Total Dose, D,} = \sum_{\substack{\text{all i}\\ \text{bins}}} D_i(\bar{E}) \times \Delta E_i \text{ ; where } \Delta E_i = \int_{\substack{\text{ith}\\ \text{energy}\\ \text{bin}}} dE$$

3.2.16 Interaction File

SAM-F provides the user with a method of calculating the production and transport of secondary gamma rays arising from neutron capture or inelastic scattering events.

During the tracking of primary source neutrons, all interactions which are capable of producing secondaries can be stored,

as an option, on an "interaction" file. The stored data are the coordinates of the collision point, the energy and weight of the primary neutron multiplied by the nonelastic interaction probability, and the time of interaction. Subsequently, this file can be processed internally by either SAM-F or SAM-A and be converted into a source of secondary gamma radiation.

3.2.17 Transmission and Escape Regions

A transmission region has the property such that when a particle enters it, the tracking of that particle is stopped and all of its parameters (x,y,z coordinates, energy, etc.) are stored on a magnetic tape called the interaction file.* In general, a transmission region is used when it is desired to run a problem in two steps.** This is usually done for very deep penetrations or for unusual geometric configurations (such as ducts) where it may be more economical to run the problem in stages. Also, the user may wish to consider several different geometries past the transmission region, but does not wish to run the first part of the problem more than once. The designation of a transmission region is, however, optional. The program is capable of treating up to 10 different transmission regions.

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* Interactions, (Section 3.2.16), and transmissions are both stored on the "interaction file".

** See Appendix R for a complete description of how this can be done.

Note that the interaction file can contain both interaction and transmission information. The 14th parameter of each particle record indicates the type of event (see Section 3.3.2 for additional information).

An escape region is one in which all particles that enter are killed. It is ordinarily, but not necessarily, used to define the outer limits of the geometry (i.e., the complete geometry is enclosed in a large region which is designated as the escape region).

3.2.18 Last Random Number Sequencer and Restart Option

Upon the completion of each statistical aggregate number of histories, the code will print out a brief intermediate edit. One of the variables printed out is the last random number sequencer. If the sequencer of the last aggregate is subsequently used as the random number sequence initiator (entered as input) for another SAM-F problem (all other input data held constant) the new computations will start where the first computation ended.

In addition, if FILE16 (aggregate scores tape) of the first computation has been saved and is available, a complete restart capability exists. The user supplies as input the history number of the last particle previously tracked, and also provides the previously created FILE16. The computation will proceed as if there had been no interruption and the final edit will provide the correct combined scores and even the correct statistics on these scores. Note that if FILE14 was used during the first run (to save interactions and/or transmissions), then FILE14, in addition to FILE16, must be supplied for the restart.

At the present time, the restart capability is available only if the internal source option is used.

3.3 Additional Descriptions of the SAM-F Program

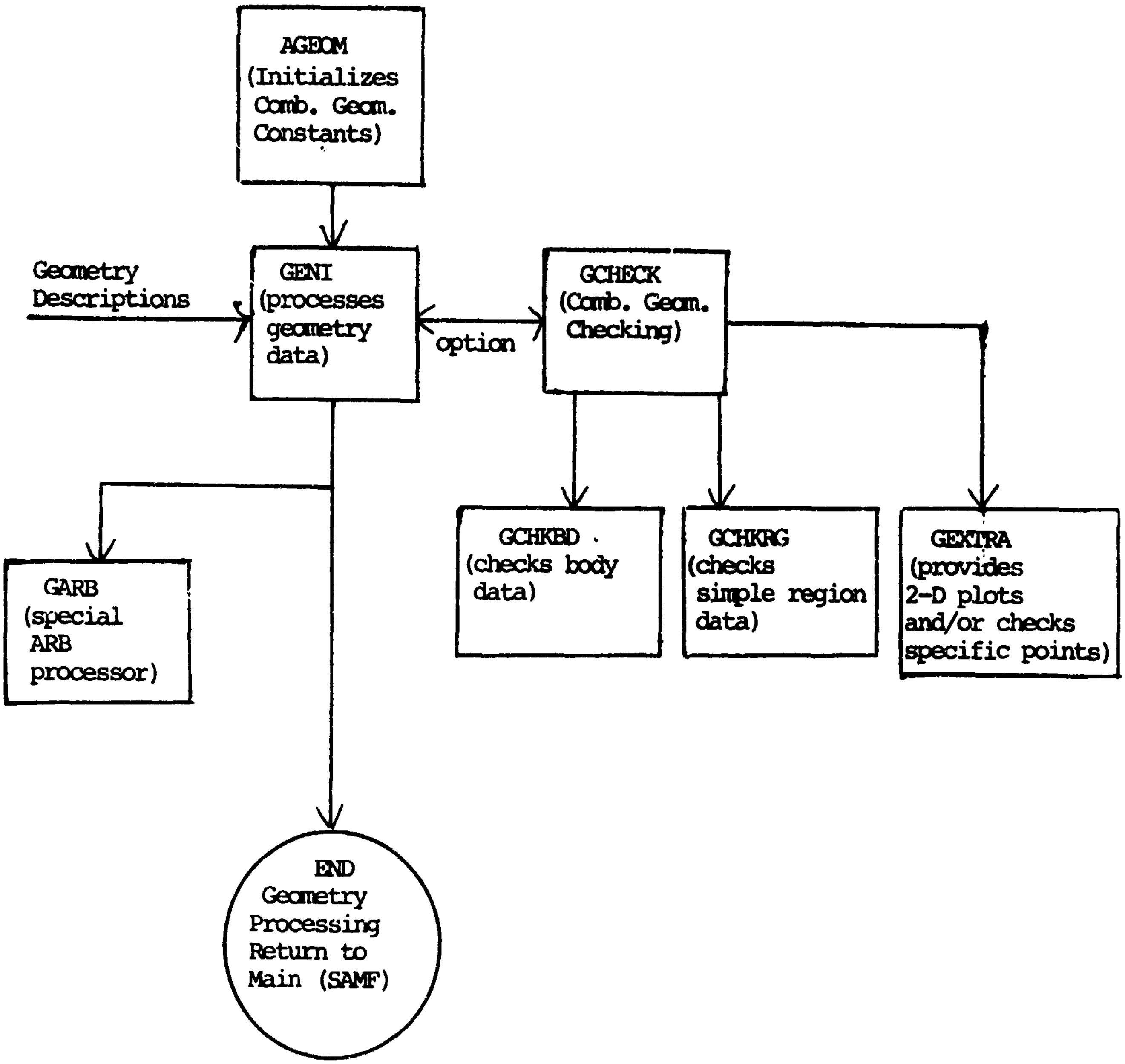
This section is included for those desiring additional organizational, mathematical and background material of the SAM-F code.

In the discussion which follows the user should refer to the next few pages.

The SAM-F program consists of a main driver (SAMF) and five primary overlays, AGEOM, ADATA, ASORTT, AMONTE, and AMOUT. AGEOM processes the geometry data. ADATA processes cross section and other input data. ASORTT sorts gamma production and neutron interaction data. AMONTE performs the Monte Carlo transport calculations. AMOUT edits the results.

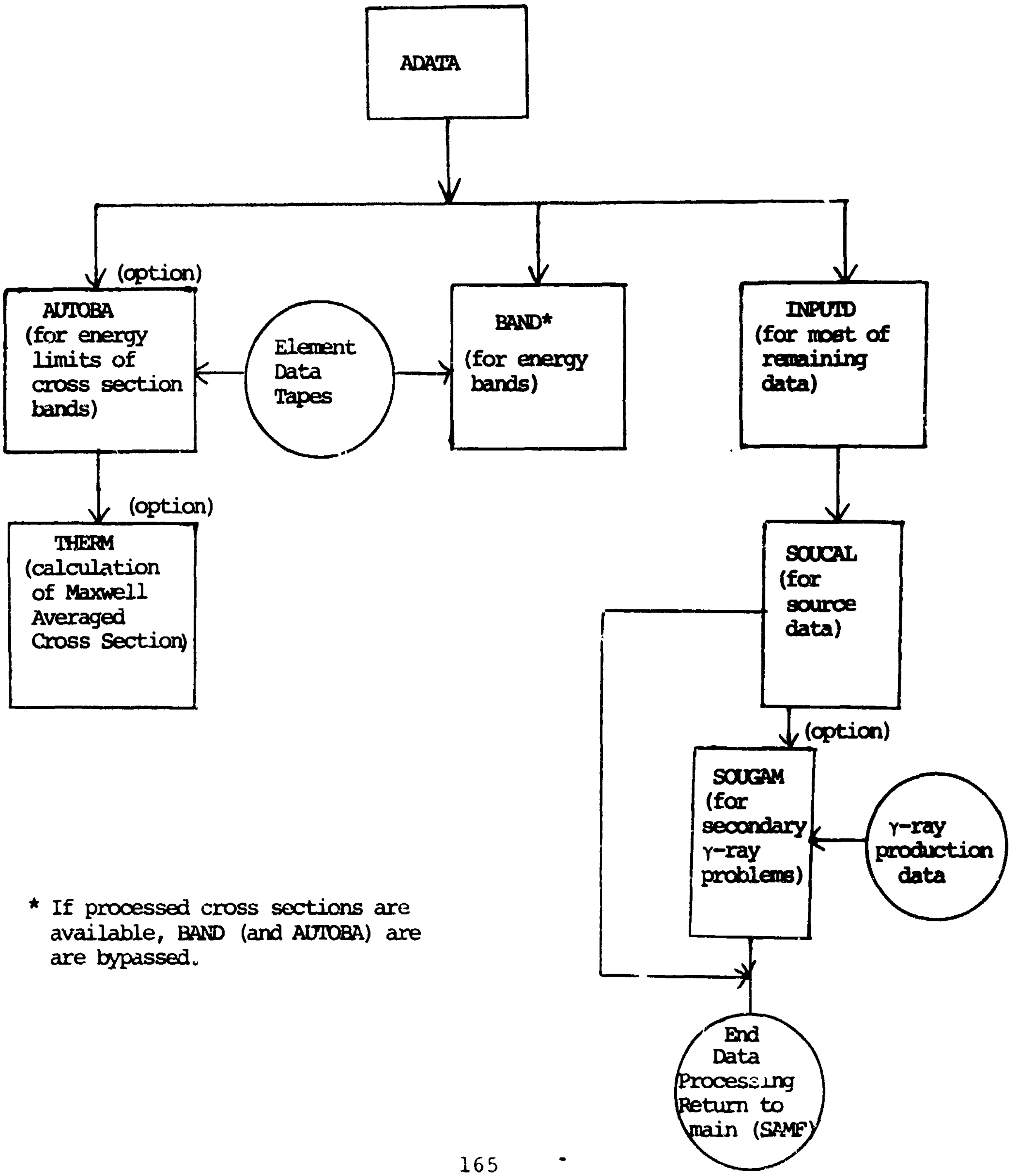
FLOW CHART (Simplified)

Overlay AGEOM



FLOW CHART (Simplified)

Overlay ADATA



* If processed cross sections are available, BAND (and AUTOBA) are are bypassed.

FLOW CHART (Simplified)

Overlay ASORTT

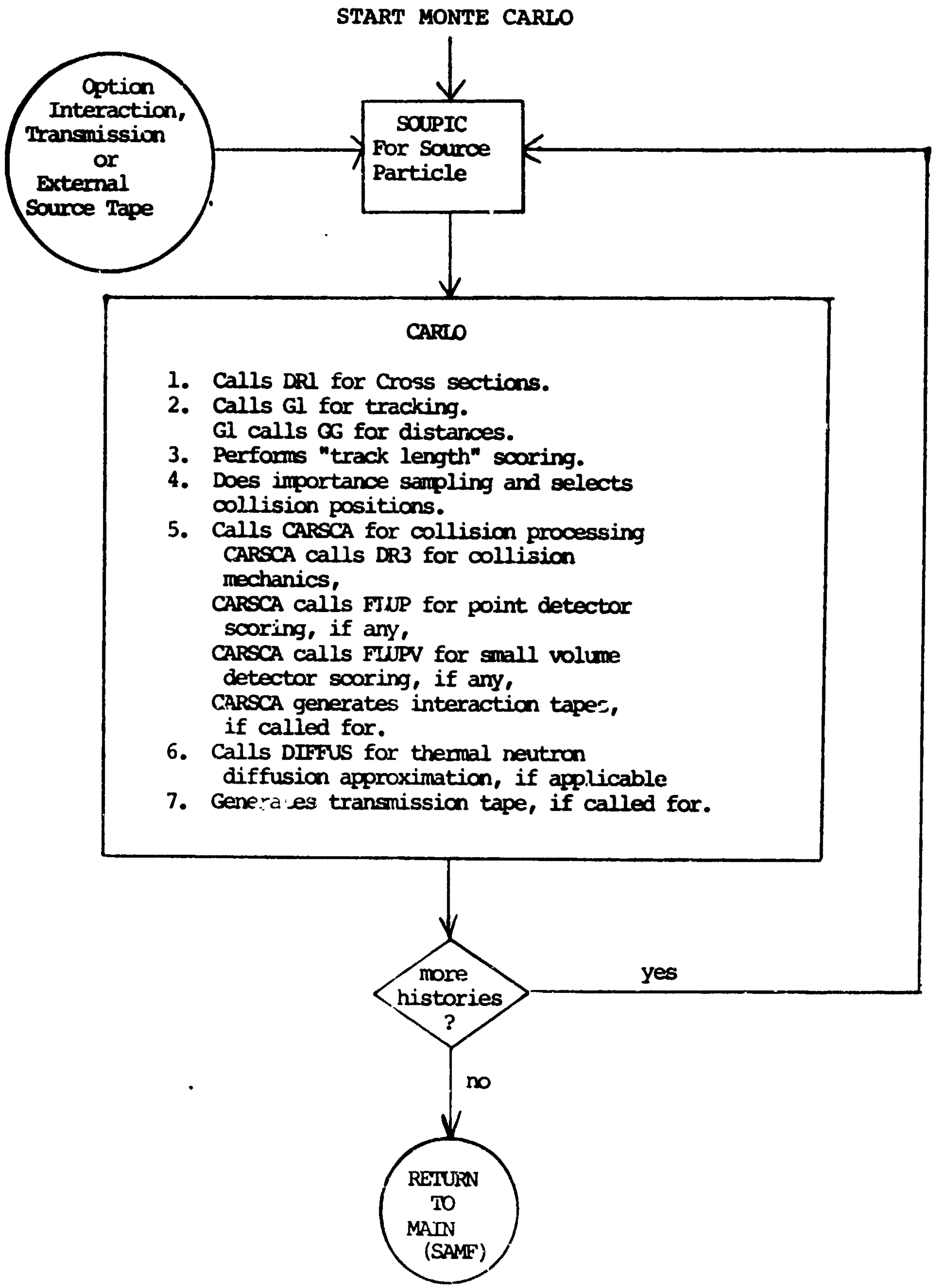
ASORTT

1. Creates an organized gamma ray production data tape (OGPDT).

2. Sorts the interaction tape, (by interacting nuclide), for each aggregate number of histories.

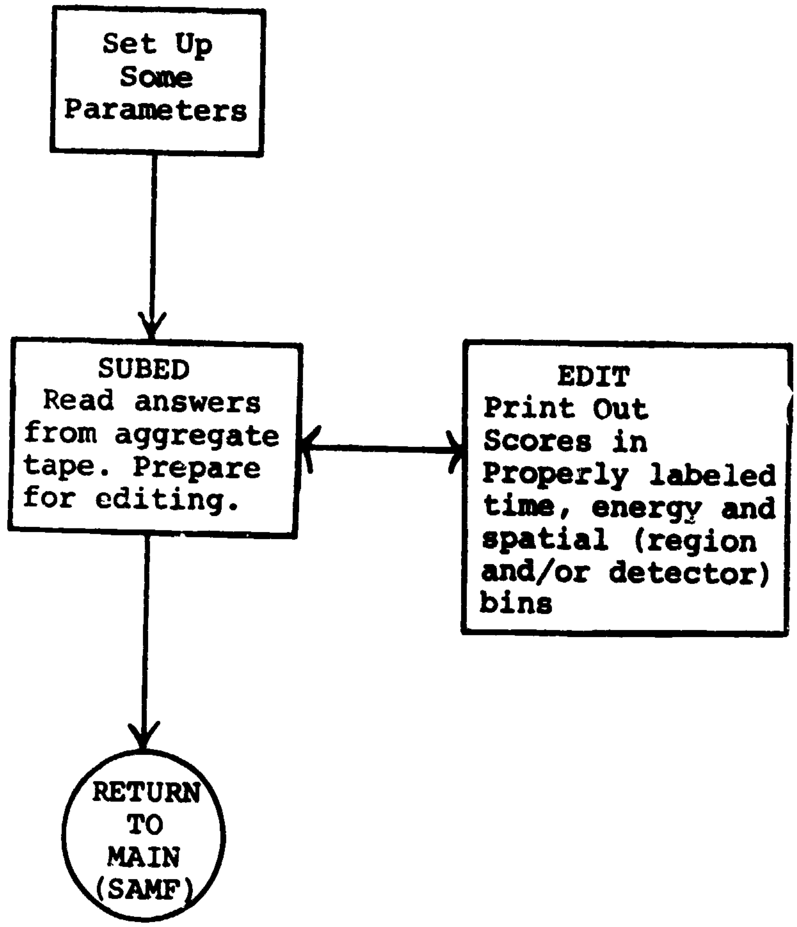
FLOW CHART (Simplified)

Overlay AMONTE



FLOW CHART (Simplified)

Overlay AMOUT



3.3.1 SAM-F Routines (Alphabetical)-General Description

This section gives a brief description of every routine in the program, given in alphabetical order. These brief descriptions are followed, in Section 3.3.2, by detailed descriptions of those important routines which are flagged by an asterisk (*) superscript.

Routine	Description
ADATA	The controlling program of the second primary overlay. It oversees three secondary overlays which read in the input data.
AGEOM	The controlling program of the first primary overlay. In this overlay, geometry data is read in and checked.
AMONTE*	The controlling program of the fourth primary overlay. It oversees the routines which generate source particles, do the tracking and scoring and perform the tallying of results. AMONTE also controls the shuttling in and out of banded cross section data and the organization of the particle histories into aggregates.
AMOUT	The controlling program of the fifth primary overlay. It calls SUBED to perform the final edit.
ANISOT	Called by DR3 to determine the center of mass angle of scattering for anisotropic events.
ARG*	The general angle reselection routine of the bounded flux-at-a-point procedure.
ARPREP	Called by ARG, as an aid in angle reselection for two special cases: (1) neutron energy just above the inelastic threshold or (2) for neutron scattering by hydrogen.
ASORTT*	The third primary overlay. For secondary gamma ray problems, this routine presorts the precursor interaction events and the production data from file 12.
AUTOBA	Calculates and supplies to BAND the energy limits for cross section bands.

BAND* The cross section processing routine. The routine reads in composition data. Element data for the required elements is read from an element data tape (EDT). The data are organized and split into bands if necessary. Composition, element, and cross section data are placed on file 10 - the organized data tape (ODT). The ODT may be saved for future calculations, if desired.

CARLO* The Monte Carlo routine which controls the tracking, importance sampling and most of the scoring and tallying of the particle histories.

CARSCA* The Monte Carlo routine which controls the interaction mechanics. CARSCA also oversees the generation of the latent tables and (option) the generation of a particle interaction tape (logical unit 14).

CHITAB An auxiliary routine for AUTOBA.

DIFIN* Precalculates some quantities for the thermal diffusion option.

DIFFU An auxiliary routine called by DIFFUS.

DIFFUS Called by CARLO to sample the thermal neutron diffusion kernel.

DIREC The routine used to compute the new direction after a scattering event.

DR1 The routine which calculates the total cross section at the present energy for the composition currently encountered by the particle being tracked. It is called by CARLO for ordinary tracking and by TRALA and TRALAV for point and small volume detector estimation, respectively.

DR3* The routine which performs the collision mechanics.

DRGE The routine which computes the probability of scattering by a given angle in the lab system. It is called by FLUP and FLUPV for point and small volume detector estimation, respectively. Moreover, it is called from DR3 when angle reselection is needed for bounded estimation.

DSPLAY Used, as an option, to display the banded cross section arrays or the gamma ray production data.

EDIT	The edit routine. It prints out flux and flux-dependent (e.g., dose) answers as functions of energy, time and scoring regions. The routine also prints out "point" and "small volume" detector results.
FILL	An auxiliary routine, called by BAND, used to fill in the cross section arrays and the scattering data tables in the banded arrays.
FLUP*	The flux-at-a-point estimation routine. The routine calculates scores as functions of energy, time, and detector point. The scores are stored in the MASTER array and are printed out by EDIT.
FLUPV*	Similar to FLUP. Used for "small volume" detectors.
GARB	Special geometry routine to process the input for the ARB body of the Combinatorial Geometry package.
GCHECK	Geometry checker routine. Calls one of four routines (GCHKBD, GCHKRG, GCHRPP or GEXTRA - see below) depending upon the type of checking being performed.
GCHKBD	Geometry checker routine. Performs various body data checks. Calls GEQUIV (see below).
GCHKRG	Geometry checker routine. Checks for simple errors in region descriptions and provides a table of region references for each body. Also, sets up proper tables in the MASTER array for subsequent geometry checking.
GCHRPP	Geometry checker routine. Once the body and simple region data have been checked by GCHKBD and GCHKRG, GCHRPP examines the RPP's placed about each body to establish possible two- or three- body overlaps. Routine GIRTWB (see below) is called for detailed checking of actual overlaps.
GCROSS	Used by checker routines to compute cross products.
GDOT	Used by checker routines to compute dot products.

GENI	The major geometry input processing routine. The routine reads geometry data, checks for some simple errors, and puts the data into the FPD and MA arrays in the form required by the tracking routines.
GEQUIV	Used by checker routines to place an RPP about each body in the geometry.
GETIR	Used to locate the region number of a given spatial location. During geometry checking it identifies points in undefined and multiply-defined regions, (see Fig. 3.5).
GEXTRA	Geometry checking routine. Calls GPOINT (see below) and also sets up the two-dimensional point grid for picture printouts.
GG	The distance calculating routine. Given a position $\overline{X}$, and direction $\overline{W}$ and a body number, the routine computes the two distances RIN, ROUT measured from $\overline{X}$ to the body.
GGTEC	Special distance calculating routine for the truncated elliptical cone (TEC).
GIROB	Until the geometry checking is complete (see GIRTWB), this routine will be used to locate points to check for possible undefined and multiply-defined regions.
GIRTWB	This routine will eventually control all final checking for undefined and multiply-defined regions. Until the location of the intersections of all body types is coded as a generalized procedure, GIRTWB checks all overlaps of body pairs where at least one of the two bodies is completely composed of planar surfaces, i.e., RPP, BOX, ARB and RAW.
GP	An auxiliary routine, called as an option by G1, for debug printout.
G1	The main geometry tracking routine. Given a position $\overline{X}$, a direction $\overline{W}$, and a region IR, the routine will calculate the distance "S" from the point $\overline{X}$ to the next region in the direction $\overline{W}$. The routine also determines IR', the next region to be encountered.
GPOINT	Geometry checker routine. Locates and prints out the region of all user-supplied points.

GRAFIC	Prints out the two-dimensional pictures.
GRID	Finds the proper region number for all points in the two-dimensional grid for picture display.
GUNIT	Used by checker routines to compute unit vector.
GVECTR	Geometry checker routine. Checks angles made by various vectors in the description of the geometric bodies.
INPUTD	Reads in most of the Monte Carlo input data and stores it in the MASTER array for use by the calculation routines. Region specification, importance sampling data, output energy meshes, and detector data are handled by this routine.
INPUTE	An auxiliary routine used to flag very distinctly all errors in the Monte Carlo input data.
LENTHS	An auxiliary routine called by BAND and FILL. Used to determine lengths of energy tables in a given energy band.
MAIN* (SAMF)	The overall control routine for SAM-F. The size of the MASTER array is set by SAMF.
NDQSET	An auxiliary function to find the length of specified arrays.
PICK*	The control routine for superbin latents. This routine stores particles whose energies are not included in the superbin currently being processed. These particles are stored by PICK in either the central memory or on tapes depending on the amount of core available for the particular problem.
RANDW	An auxiliary routine called by FILL to read binary blocks of data from the element data tape (EDT) and to write binary blocks of reduced data on the banded organized data tape (ODT).
RANF	A built-in random number generator.
REED	An auxiliary routine to read in binary arrays, or partial arrays, very rapidly.

SEEK*	Given an array, A, with elements monotonically decreasing and a variable, X, this routine will search through the A array and determine the bin containing X.
SOUCAL*	The input processor for the source information required by the Monte Carlo routines for primary transport problems. The routine processes energy and time spectra data, and source region data which are stored in the MASTER array.
SOUGAM*	The routine which generates the source particles for secondary transport problems.
SOUGEN*	The routine which generates the source particles for primary transport problems - except for the external source option.
SOUPIC*	The routine which calls either SOUGAM or SOUGEN to generate secondary or primary source particles, respectively. It will also read in source data from an external source tape. In addition, SOUPIC controls the angle of emission reselection procedure for problems involving one or more point detectors.
SOUSEC	The input processor for the gamma production data for secondary transport problems.
SUBED	The main edit routine. The routine reads the answer arrays from the statistical aggregate tape and prepares it for editing by the EDIT routine. Flux-dependent responses are also calculated in this program.
TALLY*	A summary routine. The routine prints a one line summary of results for each statistical aggregate. Quantities such as number of collisions, absorptions, and energy deposition are printed for each aggregate.
TDIFIN	Called by INPUTD if the thermal neutron diffusion option has been involved. TDIFIN reads and preprocesses the diffusion option input.
TERP	A linear interpolation routine.

THERM	A subroutine, called by AUTOBA, which precalculates cross sections averaged over the Maxwellian spectrum for the thermal neutron option.
TIMEX	Used to keep track of computer running time during Monte Carlo execution.
TRALA*	A tracking routine used by FLUP, the main flux-at-a-point routine. It tracks from an initial collision (or source) point to a detector point.
TRALAV*	Similar to TRALA. Used by FLUPV, the flux-in-a-small-volume routine.
TROPIC	A routine to generate a vector of direction cosines from an isotropic distribution.
VCALC	The volume computation routine. Region volumes are computed by numerical integration.
WRIT	An auxiliary routine to write out binary arrays, or partial arrays, very rapidly.
WRT14	A routine to write 14-word records onto tape. The routine is called whenever a transmission or interaction is to be put on tape.

3.3.2 SAM-F Routines (Alphabetical)-Detailed Descriptions

Program AMONTE

In order to help the reader understand the operation of AMONTE, a brief description of the "superbin" procedure in SAM-F is presented. It will be seen, below, that the routine BAND arranges cross sections in certain energy bands. The output energy bins (for scores) are also arranged in certain output supergroups. Cross section input corresponding to a single band can be stored in computer memory at any given time. Scores corresponding to a single output supergroup can be stored in computer memory at any given time. The two meshes (bands and output supergroups) do not necessarily coincide. A combined mesh defines a set of "superbins."

The AMONTE program starts by reading in the highest energy cross section band, and by arranging the memory for the highest energy output supergroup. The highest of the low-energy bounds of these energy ranges defines EBL, the low energy of the superbin currently treated.

The program then calls the source-picking routine SOUPIC. Upon return from SOUPIC, AMONTE examines the energy, E. If E≤EBL, the particle is stored as a latent by calling the storing portion of subroutine PICK, and SOUPIC is called again. When E>EBL, the subroutine CARLO is called. The subroutine CARLO tracks the particle scores contributions to volume fluxes when needed, and calls FLUP or FLUPV for "point" or "small-volume" detectors,

respectively. Particles coming out of collision are also tracked if their energy is above EBL; particles coming out of collision with $E<EBL$ are stored as latents by calling PICK. Control is finally returned to AMONTE which proceeds to the next source particle, until a complete statistical aggregate of particles has been treated for the highest superbin.

At this point, AMONTE switches to the next superbin by either reading a new band of cross section data, or by writing out on tape the set of scores obtained and preparing the memory layout for the next supergroup, or both. It then proceeds to call the retrieval section of subroutine PICK, which returns latents from previous superbins. IF $E\leq EBL$, the particle is stored again as a latent by calling PICK. If $E>EBL$, CARLO is called. The procedure continues until all latents have been examined, at which point AMONTE switches to the next superbin, etc., until the lowest energy superbin in the problem is finished for the present aggregate. When this occurs, AMONTE switches back to the highest superbin, and proceeds to treat the next statistical aggregate of particles. The calculation terminates when a history number exceeds the cutoff value NSTOP specified on input. A "blank" interaction record, with NSTOP=NSTOP+1, is written on the interaction tape and all tapes are rewound. Control is then transferred back to the main overlay for subsequent call to the editing overlay, AMOUT.

Subroutine ARG

This is the general angle reselection routine of the bounded flux-at-a-point estimation procedure. A non-mathematical description is given in this section.

Subroutine ARG is called by SOUPIC following a selection of source direction, or by DR3 and DIFFUS following the selection of a post-scattering direction. In either case, this initially selected direction will be reselected, if the selected ray intercepts the sphere of influence, or "critical sphere," around a "live" detector, i.e., a detector whose scoring capacity is currently active. This angular reselection procedure comprises three distinct stages: (1) direction checking; (2) reselection of angle; (3) weight adjustment.

In the direction checking stage, the orientation of live detectors with respect to the originally selected ray is analyzed. If the ray does not intersect any detectors, reselection is bypassed. If an intersection is found, reselection may be necessary, but prior to reselection, potential "conflicts" must be resolved. Two types of conflicts are possible: (1) The intersected critical sphere overlaps the critical sphere of another live detector; (2) The cone, with vertex at the collision (or source) point, which is tangent to the intersected critical sphere, overlaps the corresponding cone of another live detector. A conflict is resolved by Russian roulette, in which all but one detector is deactivated.

Subsequent to the direction checking stage, at most one live detector sphere is intersected by the originally selected ray. If such an intersection has survived, a new direction is selected in the reselection stage.

The final stage in the reselection procedure involves the calculation of a weight adjustment factor which compensates for the biasing introduced by reselection.

Program ASORTT

ASORTT re-organizes the gamma ray production data and the neutron interaction tape so as to provide (for secondary problems) a memory saving scheme analogous to the BAND feature for transport cross sections. Whereas BAND automatically splits cross section data into two or more energy ranges, to be treated one at a time, ASORTT makes provisions so that during the generation of secondary gamma rays, gamma production data for one element only resides in the MASTER array at any given time.

The basis for this memory-saving process, lies in the creation of an organized gamma production data tape (OGPDT) and a sorted interaction tape, (SIT).

The format of the OGPDT is similar to the original gamma production data tape described in Appendix D, except that:

a) the first two words for each element are dropped
b) the pointers are made relative to the starting address in the MASTER array
c) the data for each element are written as one logical record on the OGPDT.

The sorting of the SIT proceeds subsequent to the creation of the OGPDT. The sorting is carried out separately for each aggregate using the element order established for the OGPDT. If the number of interactions in an aggregate exceeds 1085, then 1085 at a time are sorted, up to a maximum of 10,850,000.

In the Monte Carlo routines, the production data for only the element currently considered need reside in memory. When an interaction for a different element is picked from the SIT, the corresponding logical record is shuttled into memory from the OGPDT.

Program BAND

The purpose of BAND is to arrange the cross section data in an organized fashion for the particular problem in process.

The basic source of neutron or gamma ray cross section data is an element data tape (EDT) generated by program SAM-X (see Appendices A and B).

The EDT contains microscopic total and partial cross sections and scattering tables (neutrons only) for all nuclides of interest. This EDT can be considered as a library tape for any subsequent Monte Carlo problems.

The BAND program first searches and reads from the EDT all information concerning the nuclides which appear in the various compositions specified in the input. It stores all data concerning these nuclides and the compositions of the program in a prescribed order. (See Appendix C.)

The output of BAND (ODT) is arranged in energy bands. The number NBAND of bands, and the (NBAND+1) band limits are derived automatically, or at the user's option, are specified on input.

The ODT consists of all cross sections and scattering tables for the high-energy band for all nuclides and compositions, followed by all cross sections and scattering tables for the next energy band for all nuclides and compositions, etc., down to the lowest energy band. (Appendix C)

Note that the gamma ray production data is not banded. Instead, overlay ASORTT is used to presort the neutron interaction and secondary gamma ray production data so that the code treats only one nuclide at a time during the generation of the secondary gamma rays.

Subroutine CARLO

This subroutine is the primary Monte Carlo subroutine of the code. Once a particle is established (in SOUPIC), its history, including all latents with energies in the current supergroup, is controlled by CARLO until termination, which, in this context also includes degradation out of the supergroup.

In order to carry out its function, CARLO uses principally three other subroutines, DR1 to obtain total cross sections, G1 to compute track lengths, and CARSCA to handle the scattering process. If the thermal neutron diffusion option is being invoked subroutine DIFFUS is also used to carry out this procedure.

In the subroutine itself, mean free path distances are calculated through the medium. Using this data, estimates of flux are made within designated scoring regions.

The Monte Carlo logic pertaining to the random selection of scattering position is carried out, using the region dependent weights for biasing. When appropriate, automatic biasing, required to bound the estimates of flux at point detectors, is also used. The following is a detailed description of the subroutine operation.

AMONTE, the controlling Monte Carlo overlay program first considers a potential new ray. This can be either a source particle (read from source tape or generated internally by subroutine SOUPIC) or a picked up latent from a previous interaction. AMONTE next tests the energy of the considered particle. If it is below the lower bound of the superbin currently treated, it is stored as a latent. If the energy of the particle is within the current superbin, it is transmitted to CARLO.

CARLO proceeds to track the particle and to score answers. Collisions made by the particle are stored by CARSCA. The tracking procedure in CARLO is as follows.

Given the region number, IR, the energy, E, and the direction of flight, $\overline{WB}$, a sampling weight*

$$W = W_{IR} \times W_E \times W_\Omega$$

is calculated. A test is made to determine whether or not the thermal diffusion option is being invoked.

If the thermal diffusion option is not being invoked, the "ordinary" tracking procedure is used. First, subroutine DR1 is called, which provides the total macroscopic cross section in the region IR.

When point detectors are being used, (and if the extended particle path passes sufficiently close to a specified detector) preliminary geometrical calculations, necessary to bias the collision positions, are carried out. This biasing is that required to make flux estimates for point detectors bounded.

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* See Appendix F or a detailed discussion of the use of the use of importance sampling in Monte Carlo calculations.

The geometry routine $G1(S_1)$ is called to provide the distance S_1 to the first region boundary encountered from $\overline{XB}$ (the current position) in the direction $\overline{WB}$. G1 also produces IR', the region number on the other side of the boundary, and $\overline{X}'$, the point of intersection of the track with the boundary. If the region IR is a scoring region, the contribution to the flux is calculated and scored. Once the tracking and scoring (if called for) are completed, the Monte Carlo procedure necessary to generate collision positions is invoked.

The general principal used for the selection of collision positions involves an implicit splitting and Russian Roulette procedure. The procedure is described in detail in Appendix Q. In summary, to select the positions, an unnormalized probability density F(s) is defined where s is distance along the track, and the expected total number of collisions is given by $G=\int_0^\infty F(s)ds$. The actual number of collisions is then either [G] or [G]+1, where the probability of the additional collision is G-[G].

In carrying out the collision dropping procedure, F(s) is treated in a piecewise fashion, where in each interval F(s) and its indefinite integral have the desired analytical properties, most important being that the indefinite integral be easily invertable. Finally to compensate for any biasing involved in using F(s), the particle weight must be adjusted accordingly.

If a collision is dropped by means of this procedure, subroutine CARSCA is called to complete the remainder of the processing. Once no more collisions positions are selected, the

subroutine proceeds. A test is made whether the next region is a transmission region (if it is, the coordinates $\bar{X}'$, IR', energy, time, etc., are written on tape)* and whether it is the escape region. If it is not an escape region, the particle tracked is moved to the boundary by setting IR=IR', by computing the new sampling weight W. Russian Roulette may be invoked to kill the particle. Next, the DR1 routine is called to obtain the new total cross section, and control is transferred to the part of the code which calls the geometry routine, G1. Thus the tracking continues until either a kill occurs or the escape region is reached. In the latter case, an estimate of "escapes" is made.

If the thermal diffusion option is invoked, subroutine DIFFUS is called to carry out the particle transport. If the region, IR, is a scoring region, volume flux estimates are made.

Note that the diffusing particle, just like the transport particle, is subject to splitting. Each split may wind up as an absorption or as an escape from the diffusion box (in which case it is stored in the regular latent table). Subroutine CARSCA is called to do all appropriate bookkeeping and to control the point detector estimation (if any).

When all splits are completed, the processing continues at the point where the latent table is under examination (see below).

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* Both interactions and transmissions are written on the "interaction" tape at the option of the user. See Sections 3.2.16 and 3.2.17.

After the tracking is completed, for either a diffusing or non-diffusing particle, the latent table of particles within the current range, is examined. If not empty, the last latent is picked up and processing continues. (Latents are created in CARSCA.) The subroutine is terminated when the latent table is exhausted.

Subroutine CARSCA

This routine controls all the necessary processing after a collision position is selected in CARLO.

DR3, is called to carry out the interaction. If the event is an absorption, the processing terminates and control is returned to CARLO.

If the event is a scattering, and flux-at-a-point (or in-a-small-volume) estimates are desired, CARSCA first calls subroutine FLUP (or FLUPV, respectively) to carry out these calculations. Next, CARSCA examines the new value of particle energy (returned, in addition to the new direction cosines, by DR3). If the energy is below the low energy cutoff, the procedure is terminated. If not, a sampling weight is calculated, and it is possible that the procedure may be terminated by a game of Russian roulette.

If the scattering event still survives it is stored as a latent in one of two latent tables depending upon whether or not the new energy lies within the range of the energy superbin currently being considered. Note that if it does fall within the current superbin and if the latent table happens to be filled up, an additional Russian roulette procedure is invoked to make more storage space available.

If an interaction tape is being created, for subsequent use as a source of secondary radiation, CARSCA will oversee the proper storing of the parameters of the interaction event. This includes both absorption and scattering events.

Subroutine DIFIN

This routine reads, as input, the coordinates and composition number of the thermal diffusion box. DIFIN then precalculates the following quantities:

(1) thermal absorption cross section

$$\mu_a = \sum_i C_i \sigma_{a,i}(ETH)$$

where C_i is the concentration (atoms/cm^3) of the "i-th" nuclide

ETH is the thermal energy (ev)

$\sigma_{a,i}$ is the microscopic absorption cross section of the "i-th" nuclide.

(2) thermal transport cross section

$$\mu_{Tr} = \mu_a + \sum_i C_i \sigma_{s,i}(ETH)(1-\frac{2}{3} A_i)$$

where $\sigma_{s,i}$ is the microscopic scattering cross section of the "i-th" nuclide

A_i is the atomic weight of the "i-th" nuclide.

(3) thermal diffusion coefficient

$$D = v/(3\mu_{Tr})$$

where v = the thermal velocity

(4) absorption mean free time

$$T = \frac{1}{\mu_a v}$$

It is recommended that the diffusion option be used in a box with dimensions of at least several transport mean free paths. The input routine actually suppresses the option if any dimension is smaller than three transport m.f.p.

It is also recommended that the sides of the diffusion box be kept a few m.f.p. away from any substantial heterogeneity.

The method of selecting a position and time to either absorption or diffusion is described in Reference 9. The selection is performed by subroutines DIFFUS and DIFFU.

Subroutine DR3

This routine performs all of the collision mechanics. The routine is called by CARSCA, to determine collision events.

A detailed description of the implementation of the scattering mechanics in SAM-F is now presented.

Elastic Scattering

Consider an elastic scattering event between a neutron with initial speed v and a nucleus at rest with mass A in units of neutron mass.

Let v' be the final neutron speed. Then if ω_L and ω_c are the cosines of the angles of scattering in the lab and center of mass, respectively, the mechanics of the event may be summarized by a velocity diagram.

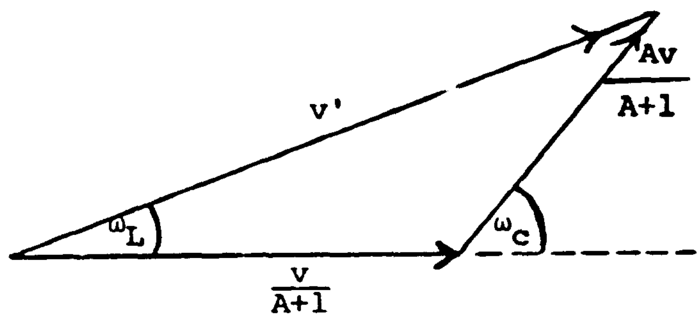


Figure 3.6 - Velocity Diagram - Elastic Scattering

Invoking the law of cosines,

$$\frac{E'}{E} = \frac{1+A^2+2A\mu_c}{(1+A)^2} \tag{37}$$

where E and E' are the initial and final neutron energies, respectively.

Inelastic Scattering

Letting Q be the exitation energy of the nucleus, the kinetic energy in the center of mass decreases to

$$\tfrac{1}{2}\mu v_r^2 = \tfrac{1}{2}\mu v^2 - Q \tag{38}$$

where μ is the reduced mass given by

$$\mu = \frac{A}{A+1} \tag{39}$$

Invoking conservation of linear momentum one obtains the velocity diagram:

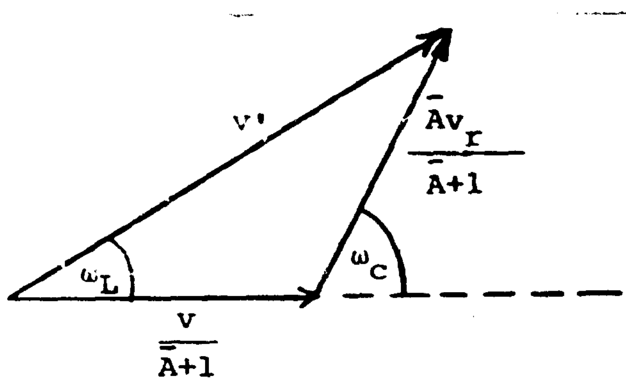


Fig. 3.7 - Velocity Diagram - Inelastic Scattering

Define an effective mass $\bar{A}$ such that

$$\bar{A} = A\, v_r/v \tag{40}$$

Equations (38), (39) and (40) yield

$$\bar{A} = A\sqrt{1-\left(\frac{A+1}{A}\right)\frac{Q}{E}} \tag{41}$$

Define v_f such that

$$v_f = \left(\frac{\bar{A}+1}{A+1}\right) v \tag{42}$$

then the triangle of Figure 3.7 is made similar to the triangle of Figure 3.6, with $\bar{A}$ and v_f replacing A and v, respectively. Consequently, the transformation analogous to equation (37) is:

$$\frac{E'}{E} = \frac{1+\bar{A}^2+2\bar{A}\omega_c}{(1+A)^2} \tag{43}$$

<u>Utilization of ENDF Information (Continuum Scattering)</u>

Current ENDF data files specify angle-decoupled secondary energy distributions expressed in the lab system after continuum scattering. This information is utilized by SAM-F as follows.

Let $\bar{E}$ be an energy sampled from the angle-decoupled secondary energy distribution. Compute $\bar{A}$ from the expressions:

$$\bar{E} = E - \left(\frac{A+1}{A}\right)Q \tag{44a}$$

$$\bar{A} = A\sqrt{\bar{E}/E} \tag{44b}$$

After sampling a cosine of scattering ω_c, the energy E' is computed from equation (43).

Averaging equation (43) over all ω_c for an isotropic distribution, one gets

$$\langle E' \rangle = E\left[\frac{1+\bar{A}^2}{(1+A)^2}\right] \quad (45)$$

Substituting equation (44a,44b) into equation (45) yields

$$\langle E' \rangle = \frac{A^2+1}{(A+1)^2} E - \frac{A}{A+1} Q \quad (46)$$

Equation (46) is consistent with the ENDF specified angle-decoupled secondary energy distribution for exitation energy Q, viz.

$$F(E \rightarrow E') = \delta\{E' - \frac{A^2+1}{(A+1)^2} E + \frac{A}{A+1} Q\} \quad (47)$$

Relativistic Energy Changes in Scattering

As shown in Appendix G, it is not necessary to consider relativistic energy changes (assuming E_{max} for neutrons is ≤ 20 Mev).

The following describes how DR3 carries out its functions.

The subroutine is called when a particle enters collision at some point within a region of given composition. Its first function is to select the nuclide in the composition with which the particle collides. The probability that a particle with energy E will intereact with nuclide k of the composition R is given by

$$P(k,R) = C(k,R)\sigma_T(k,E)/\mu_{T,R}(E)$$

where $\mu_{T,R}(E)$ is the total macroscopic cross section of the composition, and $C(k,R)$ is the concentration of nuclide k in region R.

$$C(k,R) = \frac{\rho_k}{A_k} N_o \times 10^{-24}$$

where ρ_k = density of the nuclide, k, in the composition (gm/cm^3)

A_k = its atomic weight

$N_o = 0.6023 \times 10^{24}$; Avogadro's number

By normal Monte Carlo procedure, DR3 generates a random number, ξ, and successively compares ξ with $P(k,R)$, for all values of k, until the condition

$$\xi < P(k,R)$$

is satisfied. Then the interaction is with that k-th nuclide.

Next, DR3 determines the type of interaction suffered by the particle. The probability that a particle with energy E will suffer the "i-th" type interaction with the already selected "k-th" nuclide, is given by:

$$P(i,k) = \sigma_i(E)/\sigma_T(E)$$

where $\sigma_i(E)$ and $\sigma_T(E)$ are the microscopic i-th reaction and total cross sections, respectively. As before a random number, ξ_1, is generated, and successively compared with P(i,k), for all values of i, until the condition

$$\xi_1, < P(i,k)$$

is satisfied. Then the interaction type is that of the i-th reaction.

Finally, DR3 performs the actual collision mechanics for this "i-th" reaction. The outcome will be a new energy (EPRIM), a new direction ($\overline{WP}$), the cosine of the scattering angle (CSTHT), and an integer (NCDB) denoting the type of interaction. The types of interaction are listed below. Isotropic or anisotropic refer to the scattering process in the center-of-mass system.

NCDB	INTERACTION
1	Discrete level inelastic scattering (isotropic)
2	Discrete level inelastic scattering (anisotropic)
3	Elastic Scattering (isotropic)
4	Elastic scattering (anisotropic)
5	Klein-Nishina scattering for gamma rays
6	Absorption
7	Continuum inelastic scattering (isotropic)
8	Continuum inelastic scattering (anisotropic)

Subroutine FLUP

FLUP is the subroutine which makes both the uncollided and the collided flux estimates at the specified point detectors.

If the computations involve primary radiation, present coding requires source to be either monodirectional or isotropic. Under the former condition, no uncollided estimate is made; under the latter condition AMONTE will call FLUP and uncollided flux is calculated simply by the familiar

$$\exp(-\lambda_E)/4\pi R^2$$

estimator, where λ_E is the mean free path distance (at source energy E) between the source and detector points and R is the corresponding distance. (Subroutine TRALA is the routine which calculates λ_E.) If the source particle is assigned a weight factor which is other than unity, this multiplicative factor will also be included in the estimate.

If the computations involve secondary radiation, the present coding allows for anisotropy of its production. Such anisotropy data is included on the gamma production data tape (GPDT). The uncollided estimate is then

$$\frac{g(\overline{\Omega}\rightarrow\overline{\Omega}')e^{-\lambda_E}}{R^2}$$

where $g(\overline{\Omega}\rightarrow\overline{\Omega}')$ is the probability, per unit solid angle, that the photon is emitted in the direction $\overline{\Omega}'$ towards the detector, given that the precursor interaction occurred for a primary particle traveling in the $\overline{\Omega}$ direction. For isotropic secondary production $g(\overline{\Omega}\rightarrow\overline{\Omega}')$ is, of course, $(4\pi)^{-1}$.

For calculation of the collided flux the procedure is as follows.

SAM-F employs a form of automatic importance sampling, during the transport game, to ensure that the scores at point detectors not only have a bounded variance, but, in addition, bounded estimates as well. (This is an improvement over the older once-more-collided procedure of Kalos[10], which exhibited only a bounded variance.)

The bounded estimation technique, described in detail in Appendix O, automatically biases the particle collision density in the vicinity of the detector (as part of the transport game) so that there is an effective additional weight factor proportional to R^2 (R= collision-to-detector distance). This additional weight factor will be referred to a few paragraphs below.

Once the biased collision point has been selected, and provided the collision event is nonabsorbing, the required angle of scattering (from the original direction to the direction of the detector) is computed. Let the cosine of this angle in the lab system be denoted by $\cos\theta$. DRGE, is then called to compute $g_s(\cos\theta)$, the probability, per unit solid angle, of scattering through the lab angle θ. (Note that for inelastic scattering, the code always takes into account the transformation process from the CM to lab systems.) DRGE also calculates the new energy, E'. If the new energy is below the superbin currently treated the particle is stored as a latent to be picked up and returned to this point of the coding at the appropriate later time in the calculation.

Next, subroutine TRALA is called which tracks from the collision point to the detector and computes $\lambda(E')$. The collided estimate is made at the detector. This estimate is

$$W \times \frac{g_s(\cos\theta) e^{-\lambda(E')}}{R^2}$$

where W is the overall weight factor of the particle going into collision. Note that W contains an R^2 factor (due to the automatic importance sampling referred to above and described in more detail in Appendix O). This term then effectively cancels out the R^{-2} term of the above expression. Thus, the usual problem of unbounded scores, as $R \to 0$, are, in essence, eliminated. This, then forms the basis of the bounded estimation procedure.

Note that, in general, collided flux estimates will be made at all detectors with the following exceptions:

(1) The required angle of scattering may not be allowable; i.e., $g_s(\cos\theta)=0$.

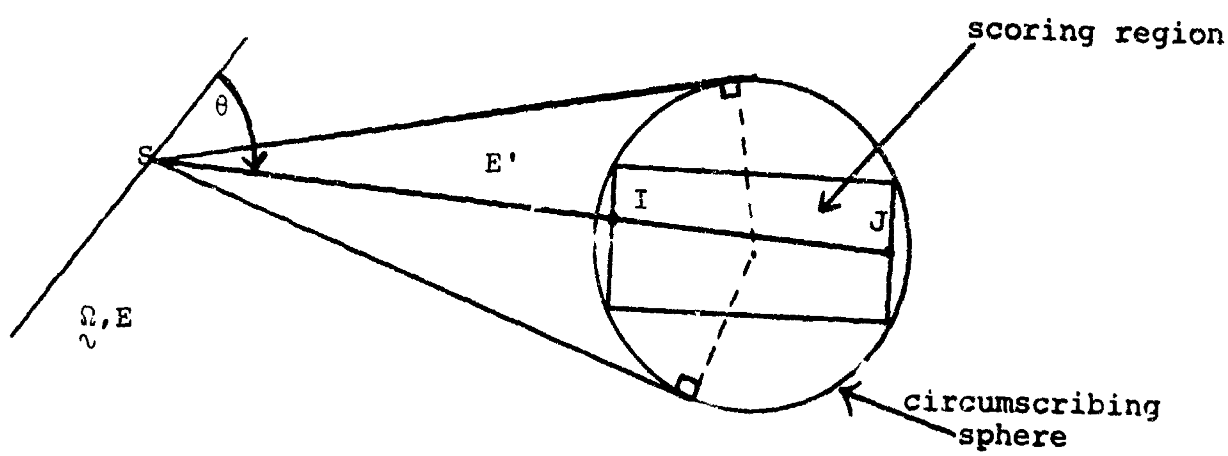
(2) As described in Appendix O, each detector is surrounded by a special imaginary spherical volume which affects the automatic importance sampling game in the neighborhood of the detector. If detectors are too close to each other, the special spheres may actually overlap. Also, the cone, with vertex at the collision (or source) point, which is tangent to the intersected critical sphere, may overlap the cone to another critical sphere. Under these conditions, a game of Russian roulette is played to determine the detector to which an estimate will be made from the current collision point.

(3) If the collision point represents a latent previously stored by FLUP (when the energy in the estimation procedure to a given detector fell below the lower limit of the then current superbin) then the estimation is made only to that given detector involved in that previous FLUP computation.

Subroutine FLUPV

FLUPV is used for the flux-in-a-small-volume option. This estimation technique is valuable for the case of a small detector, usually far from the source, inside of which the flux cannot be considered to be uniform.

At the start of the Monte Carlo calculations the code receives input describing which simple regions (sphere, box, cylinder) are to be the small volume detectors. For each, a sphere is then circumscribed about the region as seen in the figure below.



The general technique in the main Monte Carlo game for scoring from any point S, either source or non-absorption collision point, is as follows, (repeated for each small-volume detector):

1. Call FLUPV from CARSCA (or AMONTE for source particles)
2. From S, construct a cone tangent to the sphere
3. From S, select an isotropic direction restricted to be inside the cone (see mathematical description below).

   For collided particles, call subroutine DRGE to calculate g_S, the probability of scattering to the selected direction and the collided energy E'. If $g_S=0$ make no score and return to CARSCA or AMONTE. For an isotropic source do not force the ray into the cone (if the ray misses, see below, no score will be made) and set $g_S=1$.
4. If E' is less than the lowest energy of the problem no score is made. If E' is lower than the lowest energy of the current energy band the particle is stored as a latent to be picked up at a later time. In both cases control is then returned to CARSCA.
5. If $g_S>0$ and E' is in the current energy band, call TRALAV to track to I, the point of interception of the ray with the detector. TRALAV will also calculate $e^{-\lambda}$, where λ is the cumulative mean free

path flight path from S to I. If the ray misses the detector completely no score is made and control is returned to the calling program.

6. If interception is made TRALAV next calculates $\overline{IJ}$ the flight distance (cm) through the detector. Control is returned to FLUPV where a track length score of

$$WT \times g_S \times e^{-\lambda} \times \overline{I} \times \left[\frac{1-e^{-\lambda_d}}{\lambda_d}\right] \text{ for } \lambda_d > 0 \quad \text{or}$$

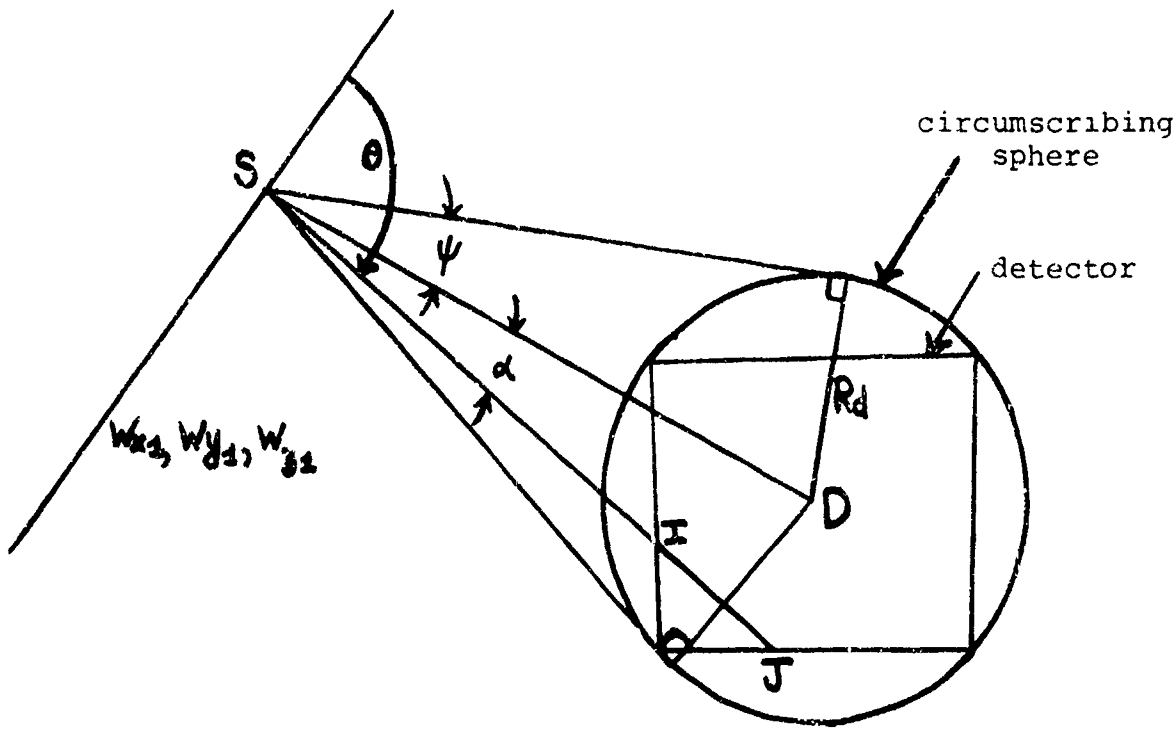
$$WT \times g_S \times e^{-\lambda} \times \overline{IJ} \qquad \text{for } \lambda_d = 0 \quad \text{(vacuum)}$$

is made, where λ_d is the mean free path flight path through the detector and WT is the weight of the particle at point S, prior to collision.

7. Note that if the ray starts inside the sphere it is allowed to scatter in an unbiased direction (non-source) or to proceed in its original direction (source) and the same estimate as above is made with $g_S=1$, and, if the particle is inside the detector as well as inside the sphere, $e^{-\lambda} \to 1$. If the particle is inside the sphere but outside the detector, and misses the detector, no score is made.

The mathematical technique to select the scattering angle at S is of some interest and is now presented.

Let the original ray have direction cosines W_{x_1}, W_{y_1} and W_{z_1} and let the coordinates of S be X_S, Y_S, Z_S.



Assume the detector is centered about point D and has a radius R_d.

S outside the sphere

$$\overline{SD} = \sqrt{(S_x-D_x)^2 + (S_y-D_y)^2 + (S_z-D_z)^2}$$

$$\cos\psi = \frac{\sqrt{\overline{SD}^2-R_d^2}}{\overline{SD}}$$

Select an angle α at random so that cos α is uniformly distributed between 1 and cos ψ, i.e., $\cos\alpha = \cos\psi + (1-\cos\psi) \times \xi$

where ξ is a random number uniformly distributed between 0. and 1.

Once $\cos\alpha$ has been selected it is simple by usual Monte Carlo procedures to select a random azimuthal angle and to calculate the direction cosines of $\overline{SI}$, which are designated Wx_2, Wy_2 and Wz_2.

Then, if θ is the selected angle of scattering:

$$\cos\theta = Wx_1 \cdot Wx_2 + Wy_1 \cdot Wy_2 + Wz_1 \cdot Wz_2$$

and

$$g_S = g(\cos\theta) \times 2\pi(1-\cos\psi)$$

where $g(\cos\theta) = \frac{1}{4\pi}$ for isotropic scattering.

S inside sphere, but outside detector

Select Wx_2, Wy_2, Wz_2 from an isotropic distribution. Then $g_S=1$ and score only if path intersects detector.

S inside detector

Again, select Wx_2, Wy_2 and Wz_2 from an isotropic distribution and then $g_S=1$.

Note: In order to increase calculational efficiency (by decreasing the number of rays which intersept the sphere but miss the detector) MAGI investigated the effects of splitting the cone into an inner and outer cone. The inner cone goes from angle 0 to $\psi/2$ and the outer cone from $\psi/2$ to ψ, (see above diagram). The code forces 3 particles into the inner cone for each particle that goes into the outer cone - with corresponding weight adjustments. This modification does seem to increase the efficiency of the technique for cubic and cylindrical detectors (with the diameter about equal to the altitude), and is currently coded in SAM-F. Investigations along these lines should continue.

Main Program (SAMF)

SAMF is the main program. After initializing some data, SAMF successively calls the five primary overlays, AGEOM, ADATA, ASORTT*, AMONTE and AMOUT to perform the geometry and cross section input processing, to reorganize the gamma production data and interaction tape*, to perform the Monte Carlo calculations and to edit the results, respectively. The size of the MASTER array is set in SAMF by the dimensioned value of MASTER in blank common. With NDQ=7,000, the entire code loads at 120,000 - 130,000 octal locations on a CDC 6600 machine; the exact amount depending on user's computer facility.

Subroutine PICK

It has been seen throughout the previous sections that particles degrading below the energy EBL, low-energy limit of the superbin currently treated, were stored as latents by calling subroutine PICK. They were later picked up by AMONTE by calling subroutine PICK. The subroutine INPUTD allocates the memory to data scores, etc. The remaining memory is assigned to the subroutine PICK, to be used as a buffer for latents. One 'end' of the buffer is assigned to 'degraded' particles. This is the end of the buffer where particles are being stored. The other 'end' of the buffer is assigned to 'unsorted' particles, i.e., the particles to be picked. Associated with each end of the buffer is a disk file to be used when the buffer overflows. There are two modes of operation. In one mode, the top of the buffer is unsorted and the bottom is sorted. When the switch is made from one superbin to the next, the 'unsorted' part is empty, and the 'degraded' part may have particles which become 'unsorted' for the superbin about to be

* Secondary gamma ray problems only.

treated. The designation of the buffers (and of the disk files) is, therefore, switched.

There is no set boundary between the two 'ends' of the buffers. The number of particles in the 'unsorted' buffer keeps decreasing, whereas the number of particles in the 'degraded' buffer keeps increasing, and can increase faster than the other number decreases. Therefore, the two parts of the buffer can meet, causing an overflow of the buffer.

It is then determined which 'end' of the buffer is longest, and a number of particles exactly equal to one-half the total length of the buffer are written from the longest 'end' onto the corresponding magnetic tape.

When the 'unsorted' buffer becomes empty, a test is made whether any 'unsorted' particles are available on the corresponding magnetic tape. If none are available, the calculation has been completed for the current superbin. If some are available, they are read into the buffer if room is available. If room is not available, it is made available by writing out part of the other buffer on the other tape; the length of the record written out from one 'end' to equal to the length of the record to be read into the other 'end'.

Subroutine PICK deals with different kinds of latents. The quantities stored are: $\bar{X}$,$\bar{\Omega}$,E,IR,T,IDET,F,NHIST,WC, and J12345, where $\bar{X}$ is the position, $\bar{\Omega}$ the direction, E the energy, IR the

region number, T the time, F the weight, NHIST the history number and WC a normalization factor. IDET and J12345 are indices.

J12345 = 1 - identifies a source particle.

= 2 - identifies a particle coming out of elastic scattering.

= 3 - identifies a particle coming out of inelastic scattering.

= 4 - identifies a latent for flux-in-a-small-volume estimation.

= 5 - identifies a latent for point detector estimation.

(in other parts of the code, J12345=2 identifies a transmitted particle and J12345=10, a nonelastic interaction.

IDET is irrelevant (set to 0) for J12345=1,2,3. For FLUP and FLUPV latents, (J12345=4 or 5), IDET is the detector number for which the latent applies. In the description of nonelastic interactions (J12345=10), IDET is a packed quantity, consisting of IATWT, a five-digit identifier of the element with which the interaction occurred, and KDLIV, used in the bounded estimation procedure (=200,000× KDLIV+SIGN(KDLIV)·IATWT).

When AMONTE calls the subroutine PICK, it examines the J12345 obtained and calls the proper routines:

J12345=1 - FLUP, FLUPV (for uncollided estimates) and CARLO

J12345=2,3- CARLO only

J12345=4,5- FLUP, FLUPV (for collided estimates)

Subroutine SEEK (For monotonically decreasing arrays)

Given the vector array, A, of length, N, and the argument "X" the routine will perform a binary search and return "I" such that

$A(I) \geq X > A(I+1); \quad I+1 \leq N.$

An error message is given if $A(1) < X$.

Subroutine SOUCAL

SOUCAL will read source data for primary transport problems and prepare tables for use by the Monte Carlo routines.

After reading in some initial descriptive data, the routine next processes data cards specifying the energy spectrum assumed to apply to all the source regions. This is a table of E vs. F(E) where

$$F(E) = \int_E^\infty S(E)\,dE.$$

Linear interpolation is assumed on E vs. $\ln F(E)$. The first entry must be for $E > E_{high}$, and the last for $E < E_{cut}$. (See Appendix E). (A monoenergetic source may also be specified).

If the Monte Carlo calculations include time dependence, the time dependence of the source must be specified. Input data cards specify tables of t vs. G(t) where

$$G(t) = \int_0^t S_t(t)\,dt.$$

Linear interpolation is assumed between entries in the table.

SOUCAL reads in this input and other kinds too, prints it back, and in general pre-computes tables to pick directly from an energy-biased source distribution. The code first pre-computes a table of

$$SPEC(I) = \int_{E_I}^\infty S(E)\,dE,$$

where the E_I's take the values of E_{high}, of all the energy boundaries where the energy weight changes, and E_{cut}. The code then runs through all the source regions, and, for each new energy-importance set encountered, pre-computes a table of

$$SPEC(I,J) = \int_{E_I}^{\infty} \frac{S(E)\,dE}{W_E(E)}$$

where J runs from 1 to the total number of different energy-importance sets encountered in the source regions; also for each angular importance set encountered, if any, a table of

$$P(I,K) = \int_{\omega_i}^{1} \frac{d\omega}{W_\omega(\omega)}$$

is computed, where the ω_i's take the values of $\cos\theta$ at which the angular weight changes, and K runs from 1 to the total number of different angular importance sets encountered. The different tables are renormalized and both the modified and unmodified integrated source are computed in each source region. The former quantities are proportional to the probability with which particles should be picked in different source regions. A table SOUR(L) is built up, which gives the cumulative probability for a source to be picked in the M^{th} region for $M \geq L$.

Subroutines SOUPIC, SOUGAM and SOUGEN

SOUPIC is used to oversee the selection of source particles from the available source distributions.

If an external source tape is to be used, groups of 35 source particles are read by SOUCAL from tape into a buffer, and returned one by one to the main code. The 14 quantities describing each external source particle are shown in Table 3.1.

If an interaction transmission tape is expected, groups of 35 interactions/transmissions are read from tape into a buffer by SOUGAM. The interaction transmission descriptions are as in Table 3.1. Secondary gamma rays are produced according to the production data, biased by region and energy as specified. Anisotropy of production can be taken into account. The angular biasing is not implemented in the generation, but only in the transport. The gamma rays are produced and returned one by one until the specified number of precursor neutron histories are exhausted or the upper limit on the number of gamma rays to be produced has been reached.

The procedure for internal source generation by SOUGEN is as follows.

A first random number ξ is compared to the table SOUR(L), (pre-computed by SOUCAL). The smallest L for which SOUR(L) $\geq \xi$ determines the region IR=ISR(L) of the source particle. Standard techniques are used to pick coordinates of points uniformly distributed in a region.

TABLE 3.1

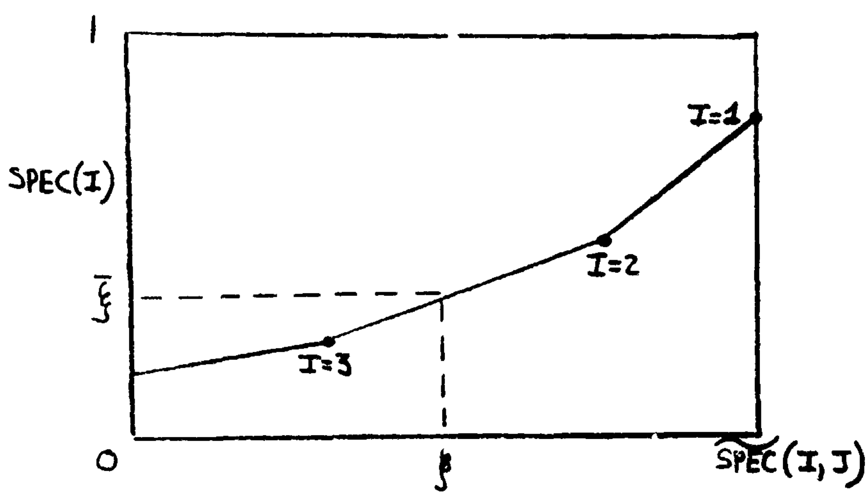
Description of 14-Word Particle Descriptive Array

WORD(s)	NAME	Stored in Latent Table (Supergroup Option Only)	Stored on External Source Tape	Interactions Stored on Interaction/ Transmission Tape	Transmissions Stored on Interaction/ Transmission Tape
1-3	$\overline{XB}$	Cartesian Coordinates	Cartesian Coordinates	Cartesian Coordinates	Cartesian Coordinates
4-6	$\overline{WB}$	Direction of Particle from the Source or Coming out of Collision	Direction of Particle from the source	Direction of Precursor Primary Particle	Direction of Precursor Particle Entering Transmission Region
7	E	Energy of Particle	Energy of Particle	Energy of Precursor Primary Particle	Energy of Particle
8	IR	Region Number	Region Number	Region Number (Must Match Precursor Run)	Region Number (Must Match Precursor Run)
9	T	Time	Time	Time	Time
10	IDET	=100x KDLIV+IDLIV if J12345=1 =IDLIV if J12345=2,3 = detector no. if J12345=4,5	Irrelevant	=200000xKDLIV+SIGN (KDLIV)xIATWT Note: = IATWT for no detectors	= IDLIV if J12345=2 = detector no. if J12345=4,5
11	F	Statistical Weight	Statistical Weight	Statistical Weight	Statistical Weight
12	NHIST	History Number	History Number	Precursor Primary Particle History Number	Precursor Primary Particle History Number
13	WC	= particle weight if J12345=1,2,3 = distance to detector if J12345=5 is ignored if J12345=4	Carry-Along Weight	Carry-Along Weight	= particle weight if J12345=2 = distance to detector if J12345=5 is ignored if J12345=4
14	J12345	= 1 for source particle = 2 for particle coming out of elastic scattering = 3 for particle coming out of inelastic scattering = 4 for small-volume latent = 5 for point detector latent	1	10	= 2 for real track transmission = 4 for small-volume estimate transmission = 5 for point detector estimate transmission

The energy is picked next. A stratified random number (called CE in the code) is obtained (stratification is done for each statistical aggregate of source particles). A biased random number ξ is then obtained by interpolation in the SPEC(J) vs. $\widetilde{\text{SPEC}}$(I,J) tables pre-computed by SOUCAL. (The J is determined by the region number.) Finally, the energy is determined by solving the equation

$$\bar{\xi} = \int_E^\infty S(E)\,dE$$

using semi-log interpolation.



The direction $\overline{WB}$ of the source particle is determined as follows: If the source is isotropic and there is angular importance sampling, the cosine of the angle between the particular aiming angle and the direction is chosen by picking a random number, and interpolating between the angular mesh supplied on input vs. the table P(I,K) pre-computed by SOUCAL. (The K is determined by the region number.) A random azimuth is then picked, which completes the specification of the direction.

In the absence of angular importance in the source region, standard techniques are used. The case of monodirectional source also can be handled, provided there is no angular importance in the source region. Finally, if time dependence is to be determined, a time T is determined by another random number ξ and the solution of the equation

$$\xi = \int_0^t S_t(t)dt$$

The quantities communicated to the main code are shown in Table 3.1.

Subroutine TALLY

The routine is used to print a tally at the end of each statistical aggregate and to print a tally by region at the end of the problem.

At the end of each aggregate the following items are printed.

NHIST	Total number of histories thus far
NCOL	Total number of collisions thus far
NTMDG	Total number of time cutoffs and degrades thus far
NABS	Total number of absorptions thus far
NESC	Total number of escapes and Russian Roulette kills thus far
ENDEP	Total energy deposition thus far
CUT	Total weighted number of escapes, absorptions, time cutoffs and degrades thus far
T	Elapsed time thus far
JCOUNT	Total number of particles on the interaction/transmission tape.
LRN	Last Random Number Sequencer (see Section 3.2.18)

For secondary transport problems, NHIST refers to precursor primary histories. For restart problems, all items except NHIST are the totals since restart.

Items 2-7, above, are also printed at the end of the problem as a function of region.

<u>Subroutine TRALA</u>

Used for flux-at-a-point.

Given an initial point $\overline{XB}$ and a direction $\overline{WB}$, the routine will track from $\overline{XB}$ in the direction $\overline{WB}$. The tracking will continue until the distance "R" measured from $\overline{XB}$ is reached.

During the tracking, the routine will form

$$AMDA = \sum_i R_i \mu_i$$

Where R_i is the geometric thickness of region "i" and μ_i is the total macroscopic cross section of region i. The quantity AMDA is the number of mean free paths along the line segment from $\overline{XB}$ to $\overline{XB}+(\overline{WB})\cdot(R)$.

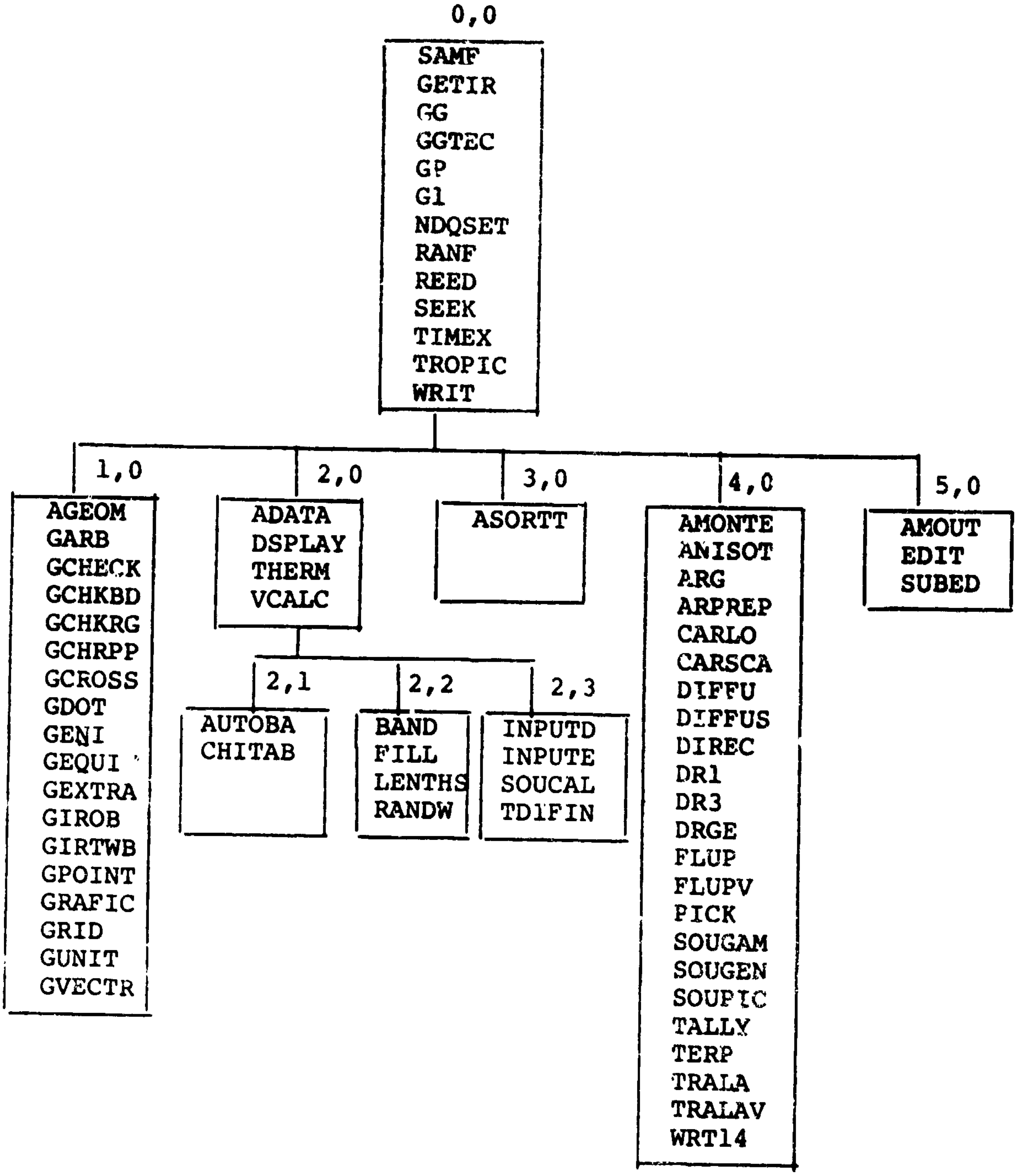
<u>Subroutine TRALAV</u>

Used for flux-in-a-small-volume.

Similar to the TRALA except that AMDA refers to the track length (mean free paths) from $\overline{XB}$ to the detector volume, and R is the track length (cm) through the detector.

3.3.3 Overlay Structure of SAM-F

The following is the overlay structure of SAM-F.



3.3.4 Glossary of Important Common Arrays

The following is a description of each variable in blank COMMON and in some of the more important labeled common arrays.

"Blank" Common

EOUT(100)	An array containing the output energy bins for flux results. The aray contains all bins for all output supergroups.
EWTAB(50)	The energy mesh for energy importance sampling.
ANGLE(50)	The cosine mesh for angular importance sampling.
TTAB(50)	The time mesh for time dependent problems.
MASTER(7,000)	The master storage array containing input and flux data. A complete description appears in Appendix H. The array is equivalenced with array ASTER.
KDUM	Dummy variable needed by function NDQSET to change the memory allocation for the MASTER array.

COMMON REGPAR

ISC	The scoring region number for region IR.
NREG	The composition number for region IR.
IRW	The location, in MASTER, of the energy weight for region IR.
IEW	The location, in MASTER, of the energy weight table for region IR.
IAM	The location, in MASTER, of the aiming angle for region IR.
IANG	The location, in MASTER, of the angular weight table for region IR.

Common INPUT

NSTART	If the expected real running time (seconds) after two additional aggregates exceeds NSTART the code will terminate the Monte Carlo and edit.
NSTOP	Number of the last history to be treated.
NSTAT	Number of histories per statistical group.
NRMAX	Number of regions in the geometry.
NG	Either 0 for a neutron problem or 1 for a gamma problem.
NT	Number of output time bins.
NOUT	Number of output energy bins.
NUMSC	Number of flux scoring regions.
NRWL	Number of distinct region weights.
IREX	The escape region number.
NEWL	Number of energy bins for energy weighting.
NEW	Number of distinct energy weight sets. If NEWL and NEW=0, the problem contains no energy weighting.
NAIML	Number of distinct aiming angles.
NUMANL	Number of angular bins for angular weighting.
NUMANG	Number of distinct angular weight sets.
JRT	Not used.
ECUT	Low energy cutoff (ev). Tracking of a particle is terminated if its energy degrades the problem.
ETHERM	Thermal energy if a thermal group is required. ETHERM must be within the energy limits of the problem.

TCUT	Time cutoff.
FZ	See discussion in Section 3.2.10.
EHIGH	High energy cutoff (ev). This should be less than or equal to the highest energy for which cross sections are available.
EBL	Lower bound of the current supergroup (ev).
EBH	Upper bound of the current supergroup (ev).

<u>Common PAREM</u>

XB(3)	The X,Y,Z coordinates of the current particle's starting point (cm).
WB(3)	The direction cosines of the current particle.
E	Energy of the particle (ev).
IR	Region number of the particle.
T	Time of flight of the particle.
IDET	A detector number used in detector calculations.
F	Importance sampling parameter.
NHIST	Current history number.
WC	An extra "carry-along" weight parameter.
J12345	A particle type flag (see the discussion of PICK).
WP(3)	Direction cosines of particle after scatter.
XP(3)	X,Y,Z coordinates of current position (cm).
EPRIM	Energy after scatter (ev).
ATWT	Atomic weight of scattering element.
NCDB	Interaction type indicator (see discussion of DR3).
CSTHT	Cosine of scattering angle.
U	Total macroscopic cross section at energy E for region IR.

LCHI	Not used.
IATWT	Identification digit of the scattering element.
IERR	Error indicator.
IDBG	Debug printout flag.
IRPRIM	Next region to be entered by the ray.
NASC	A flag to initiate the 'G1' routine for a new ray.
LSURF	Not used in Monte Carlo. In geometry package it refers to the number of the intersected surface.
NBO	Not used in Monte Carlo routines. In geometry package it refers to "body number".
LRI LRO RIN ROUT KLOOP LOOP ITYPE PINF NOA DIST	Geometry subroutine parameters.

<u>Common COMPUT</u>

NUMNOU	The product of NUMSC (the number of scoring regions) and NOUT (the number of output energy bins).
JONUM	An index used in flux scoring.
LNCOL	The location in MASTER of the collision by region table.
LENDEP	The location in MASTER of the energy deposition by region table.

LREGT	The location in MASTER of the region data table.
LNESC	The location in MASTER of the escapes by region table.
LCUT	The location in MASTER o the weighted number of escapes, absorptions t. cutoffs and energy degrades by region table.
LLAST	The location of last word in MASTER used by the program.
NDQ	The size of the MASTER array*
LNTMDG	The location in MASTER of the time cutoff and degrade by region table.
LNABS	The location in MASTER of the absorption by region table.
LSCORE	The location in MASTER of the flux scoring array.
LPACK	Not used.
NTOT	NUMSC times (the number of energy bins in the largest supergroup).
LGEOM	Not used.
LEGEOM	Location prior to start of output storage in MASTER array.
KSOUR	Last location in MASTER array prior to source data.

<u>Common FAP</u>

XAD(25)	The array of X-coordinates for the detectors.
YAD(25)	The array of Y-coordinates for the detectors.
ZAD(25)	The array of Z-coordinates for the detectors.
IDD	The number of the detector being processed.
NDFAP	Not used.
NDET	The total number of detectors.
LSCFAP	The location in MASTER of the scoring array for detector fluxes.
LPAFAP	Not used.

---

*To alter size of MASTER/ASTER array, change dimensions in MAIN program.

3.4 Input, Output and Tape Assignments

3.4.1 Input Formats

Definitions of all input quantities and corresponding card formats are given below. The definitions are given in the order in which the data are required by the code.

Items 1-10 pertain to the Combinatorial Geometry input and checking.

Items 11-15 pertain to the cross section treatment and several debug printout options.

The remaining items pertain to the Monte Carlo process input.

(In filling out input the user may wish to refer to Appendix E which displays the hierarchy of all input energy limits and tables.)

3.4.1.1 Geometry Input

Item 1 General Information (Format 4I5,E15.5,A1,11A4)

IGOPT	= 0, Suppress both geometry checking and picture taking options
	= 1, Check for body and region description errors
	= 2, Make picture(s) of plane slices(s) through the geometry and/or check user-specified points
	= 3, Do both 1 and 2
IESC*	Escape Region. (See also footnote 2.)
IORPP*	= 0, During geometry checking, suppress full RPP overlap printout
	= 1, During geometry checking, provide full RPP overlap printout
IPRINT	= 0, Print out body and region data which follow
	= 1, Print out body and region data as well as the internal arrays in which they are stored
	= 2, Suppress all geometry printout
SCALE	Scale Factor. Multiply all Combinatory Geometry dimensions by this factor. (Default = 1.0)
MA	Title, 45 arbitrary Hollerith characters

---

* These items need be entered only if IGOPT = 1 or 3. Otherwise, they may be left blank.

** The escape region is a special region which generally encloses all other regions. In the ray-tracing part of the code, rays entering the escape region are terminated.

Item 2 Body Cards (Format 2X,A3,1X,A4,6E10.3)

The computer assigns to each body an ordinal number which depends on the order in which the body cards are read in. Therefore, it is most important that the card sequence match the numbering sequence.

Nine different body types may be employed. The standard format for each body is as follows.

Columns	Input
1-2	Arbitrary (not read in)
3-5	Three-letter body identifier
6	Arbitrary (not read in)
7-10	Four characters of arbitrary Hollerith data (not required)
11-70	Divided into six floating point fields of 10 columns each. Body dimensions are given here in centimeters.

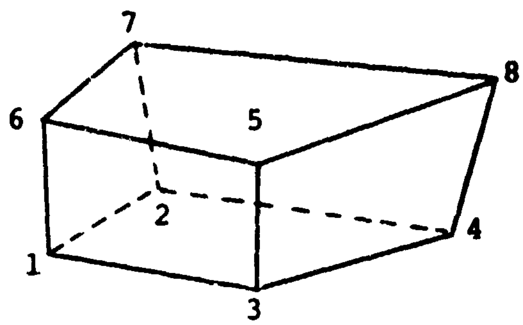
Table 3.2 describes the input required for each body. The quantities V, H, etc., were defined in Section 3.2.1.2.

Note that the last card of the body data must be END punched in columns 3, 4, 5. This is the signal that all body data has been treated.

Body Type	3-5 3-letter ID	Card Columns 11-20	21-30	31-40	41-50	51-60	61-70	Number of Cards Needed
Rectangular Parallelepiped	RPP	X_{min}	X_{max}	Y_{min}	Y_{max}	Z_{min}	Z_{max}	1
Box	BOX	Vx H2x	Vy H2y	Vz H2z	H1x H3x	H1y H3y	H1z H3z	1 of 2 2 of 2
Sphere	SPH	Vx	Vy	Vz	R	-	-	1
Right Circular Cylinder	RCC	Vx R	Vy -	Vz -	Hx -	Hy -	Hz -	1 of 2 2 of 2
Right Elliptical Cylinder	REC	Vx R1x	Vy R1y	Vz R1z	Hx R2x	Hy R2y	Hz R2z	1 of 2 2 of 2
Ellipsoid	ELL	V1x L	V1y -	V1z -	V2x -	V2y -	V2z -	1 of 2 2 of 2
Truncated Right Cone	TRC	Vx R1	Vy R2	Vz -	Hx -	Hy -	Hz -	1 of 2 2 of 2
Right Angle Wedge	RAW or WED	Vx H2x	Vy H2y	Vz H2z	H1x H3x	H1y H3y	H1z H3z	1 of 2 2 of 2
Arbitrary Polyhedron	ARB	V1x V3x V5x V7x	V1y V3y V5y V7y	V1z V3z V5z V7z	V2x V4x V6x V8x	V2y V4y V6y V8y	V2z V4z V6z V8z	1 of 5 2 of 5 3 of 5 4 of 5
		Face Descriptions (See Note on following page)						5 of 5
Truncated Elliptical Cone	TEC	Vx Nx R1	Vy Ny R2	Vz Nz P	Hx Ax -	Hy Ay -	Hz Az -	1 of 3 2 of 3 3 of 3

TABLE 3.2 - INPUT REQUIRED FOR EACH GEOMETRIC BODY TYPE

Note: Each of the six faces of an ARB are described by a four-digit number giving the number of the four vertex points at the corners. The order of specification of the four points is completely arbitrary. The point specification format is 6(F10.1) starting in Column 11. An example is shown below.



FACE	1	2	3	4	5	6
PTS	1653.	3548.	4278.	1762.	1243.	5678.

When the number of faces is less than six, the remaining face description(s) must be zero, and must appear at the end of the list.

If a face has three vertices, the omitted position may be either 0 or a repeat of one of the other vertices.

Eight vertices must always be supplied. Those that do not appear in face descriptions are ignored.

Item 3 Region Cards (Format 2X,A3,5X,9(A2,I5))

Each region must be numbered and described by a logical combination of the bodies which make up that region. Use as many cards as necessary to describe each region and begin each region on a new card.

Columns	Input
1-2	Blank
3-5	Arbitrary non-blank Hollerith Data
6-10	Blank
11-12	Insert (OR) if needed. Otherwise, leave blank.*
13-17**	Body number preceded by either the "+" or "-" operator.
18-73	Divided into eight fields, each being similar to Columns 11-17. The first two columns of each field are reserved for the OR operator, if needed. The last five columns are for the body number preceded by either the "+" or "-" operator.

Use as many cards of the above type as needed to complete a region description, but leave Columns 1-10 blank on all continuation cards.

The last region description card must be followed by a card containing an END in Columns 3, 4 and 5. This informs the code that all regions have been described.

* For SAM-F, the source region(s), see item 34, must precede sequentially any region which is described by the (OR) operator. For SAM-A, the detector region, (see Section 4.4.1), must precede sequentially any region which is described by the (OR) operator.

** Default Option (blank entry) for operator is "+".

NOTE: If IGOPT (of Item 1) = 0 or 1, Omit Items 4-10

Item 4 Picture Display Option (Format 2I5)

NUSE,NBRK — Two flags to control character set used in picture displays:

NUSE=0; (NBRK ignored) - The standard 46 character set is used (see Item 5 for description). This will cycle every 46 regions

46≥NUSE>1; NBRK=0 - The first NUSE standard characters will be replaced by the NUSE entries of Item 5. The new character set will cycle every 46 regions.

46≥NUSE>1; NBRK≥NUSE≥1

(a) For region numbers ≤NBRK, the character set will cycle every (NUSE-1) regions

(b) For region numbers >NBRK, the NUSE character is always used.

NOTE: If NUSE = 0, Omit Item 5

Item 5 Character Set (Format 46A1)

ATABLE(I), I=1,NUSE: The list of characters that are to be printed for each region. If N≥47, the character is Modulo (46) e.g., N=48 is the same as N=2.*

The standard default values of ATABLE are:

Region Number	Character Printed
1 through 9	1 through 9
10	0 (zero)
11	A
12	B
13	C
14	D
15	E
16	F
17	G
18	H
19	I
20	J
21	K
22	L
23	M
24	N
25	O
26	P
27	Q
28	R
29	S
30	T
31	U
32	V
33	W
34	X
35	Y
36	Z
37	+
38	-
39	*
40	/
41	(
42	)
43	=
44	.
45	,
46	(blank)
≥47	Modulo (46)

* Unless NBRK of Item 4 is >0. Then the character is Modulo (NUSE-1).

Item 6 Option Card (Format 2I5)

IOPT1	>0	Will read in, and locate the region of, IOPT1 specified points
	=0	Will suppress this option
IOPT2	>0	Will take IOPT2 pictures of the geometry
	=0	Will suppress this option

> NOTE: Enter Item 7 IOPT1 times.

Item 7 Specified Points (Format 3E12.4)

XB(I),I=1,3 — Enter the Cartesian coordinates (cm) of each IOPT1 point to be tested

> NOTE: Repeat Items 8-10, IOPT2 times

Item 8 Picture Boundaries (Format 6E12.4)

X_{UL}, Y_{UL}, Z_{UL} — X, Y, and Z coordinates in the combinatorial geometry of the upper left corner of the picture.

X_{LR}, Y_{LR}, Z_{LR} — X, Y, and Z coordinates in the combinatorial geometry of the lower right corner of the picture

NOTE: Item 8 partially describes the plane of the slice by defining two points in the plane and designates the top, bottom, left and right sides of the picture. The picture must not enter into the "escape region" (see Item 1).

Item 9 Direction Cosines (Format 6E12.4)

$\left.\begin{matrix} U_X \\ U_y \\ U_Z \end{matrix}\right\}$ Direction numbers proportional to the direction cosines for the U axis of the picture. The U axis points down the printed page in the direction the page moves through the printer. (Note: if the Z-Axis is parallel to the edge of the paper and positive Z is upwards, use (0.,0.,-1.) for (U_x,U_y,U_z).)

$\left.\begin{matrix} V_X \\ V_Y \\ V_Z \end{matrix}\right\}$ Direction numbers for the V axis of the picture. The V axis points to the right across the page.

NOTES: 1) The U and V axes may have arbitrary orientation. However, if they are not orthogonal the resulting picture will be distorted.

2) Item 9 completes the description of the plane of the slice by giving a line in the plane. It also specifies the orientation of the picture on the output.

Item 10 Grid Spacing (Format 2I5,2E10.5)

NU: Number of intervals to print along the U axis (overrides DELU).

NV: Number of intervals to print along the V axis (overrides DELV).

DELU: Spacing (in centimeters) of intervals along the U axis.

DELV: Spacing (in centimeters) of intervals along the V axis.

NOTE: All four entries are not required as input. See explanation which follows.

Additional Comments on Item 10

Either NU or DELU can be used to specify the spacing along the U axis. If both are given, NU will override DELU.

Similarly, either NV or DELV can specify the V axis spacing with NV overriding DELV.

If both the U axis spacing and V axis spacing are specified by the user, the picture will be distorted (perhaps intentionally) unless DELV=0.6X DELU. This is because standard printers give 10 characters to the inch across a line but only 6 lines per inch down the page.

As an aid to the user, if only the U axis spacing (or the V axis spacing) is specified, the code will automatically set the other axis spacing so that DELV=0.6XDELU. The picture generated will thus be undistorted.

The simplest method to obtain the correct results is to specify two diagonal corners of the plane of the slice on Item 8, with the top having the short dimension, if it is not square, and the side having the long dimension. Then, on Item 9, specify the U axis to be parallel to the edge of the slice with the large dimension (left or right side), and the V axis to be parallel to the edge of the slice with the small dimension (top or bottom). Finally, let the only entry on Item 10 be NV equal to the maximum number of characters per line on your printer; this will provide the largest undistorted picture.

The authors usually set NV to 130 and leave the rest of Item 10 blank.

3.4.1.2 Cross Section Input

Item 11 Option and Title Card (Format 4I3,2(2X,L1),A2,15A4)

IODT - cross section energy banding option

= 0, do energy banding of cross sections

= 1, energy banding previously done; output must be available on logical unit 10.

IBEDT- band edit option (applicable only if IODT=0)

= 0, do not display energy banded cross section arrays

= 1, do display energy banded cross section arrays

NBAND- number of energy bands in which the cross sections are to be processed. Use NBAND=0 for automatic banding or for banding previously done and available as Tape 10. During tracking, the cross sections in only one band are in the computer at any one time. (NBAND≤49.)

IDBG - debug printout for tracking of particles

= 0, no printout

= 1, main debug printout option

= 2, same as IDBG=1 plus much extra geometry tracking printout

= 3, same as IDBG=1 plus gamma ray production data printout

= 4, same as IDBG=2 plus gamma ray production data printout

SSDR1= 0 (or F) no debug printout from subroutine DR1

= T debug printout from subroutine DR1

SSDR3= 0 (or F) no debug printout from subroutine DR3.

= T, debug printout from subroutine DR3.

NAME Title; any 62 arbitrary Hollerith characters

NOTE: If NBAND=0, omit Item 12.

Item 12 Cross Section Band Limits (Format 5E15.6)

Enter the energy limits (in ev) of each band starting with the highest energy and proceeding to the lowest energy. There must be NBAND+1 entries, using as many cards as necessary. The energy bands must exceed the energy range from EHIGH to ECUT (see Item 21 below).

NOTE: If IODT (of Item 11)=1, omit Items 13,14 and 15.

Item 13 Composition Identification (Format I10)

NCOMP - total number of compositions in the problem.

NOTE: Repeat Items 14 and 15 for each (NCOMP) composition.

Item 14 Number of Elements (Format I10)

NE - number of nuclides in present composition (≤ 10).

NOTE: Repeat Item 15 for each (NE) nuclide in present composition.

Item 15 Element Card (Format 10X,I10,E15.6)

ID - an integer which identifies the nuclide (5 decimal digits ZZAAA)

ZZ = atomic number

AAA = truncated atomic weight for a nuclide

= 000 for a naturally occurring mixture of isotopes

CONC - atomic concentration of nuclide in this composition in units of 10^{24} atoms/cm^3.*

---

* Calculate by multiplying weight density in material (grams/cm^3) by $\frac{.6023}{A}$, where A = non-truncated atomic weight and .6023 = Avogadro's Number in units of 10^{24} atoms/gm. For a vacuum description, [illegible] vanishingly small, but nonzero, concentration, for example, 1.E-10.

3.4.1.3 Monte Carlo Input

Item 16 Start/Restart Information (Format I20,I10)

LRN*	Number to initiate random number generator (see Section 3.2.18). If zero (or blank), the default option (=1) will be used.
IRSTRT	Number of histories previously processed. =0 New computation; calculations start at history 1 >0 Restart; calculations start at history IRSTRT+1 and previously generated logical file 16 must be available.

Item 17 Statistical Data (Formats 3I10,8I5)

NSTART	The number of real time seconds of running time before terminating and editing.**
NSTOP	Number of the last history to be treated.
NSTAT	Number of histories per statistical group.
NRMAX	Number of regions in the geometry.
NG	Enter 0 for a neutron problem or 1 for a gamma problem.
NT	Number of output time bins (enter 0 for a time-independent problem). ($\leq$50)
NOUT	Number of output energy bins. ($\leq$100)
NUMSC	Number of flux scoring regions. ($\geq$1)
NRWL	Number of distinct region weights.
IREX	The escape region number.
JPRINT	=0, print out Monte Carlo input data =1, suppress all but a limited amount of Monte Carlo input data printout.

---

* For restart option LRN should be equal to the final (printed-out) value of LRN in the previous run. As a convenience, the code will automatically set LRN to this value if LRN is entered as zero (or blank).

** Upon completion of each statistical aggregate the code estimates the total (real) running time at the end of two additional aggregates. If this time exceeds NSTART (seconds) no new aggregates will be started and control is switched to the edit overlay, AMOUT.

Item 18 Transmission-Interaction Information (Format 10I5,2I10)

IRT(1) IRT(2) IRT(3) IRT(4) IRT(5) IRT(6) IRT(7) IRT(8) IRT(9) IRT(10)	Transmission region numbers. Leave blank if no transmission region.
IWE (col.60)	Enter a "1" if neutron elastics or photon Compton scattering events are to be recorded on tape, otherwise leave blank.
IWO (col.70)	Enter a "1" if absorptions and neutron inelastics are to be recorded on tape, otherwise leave blank.

Item 19 Number of Detectors (Format 2I10)

NDVOL *	Total number of flux-in-a-small volume detectors. (NDVOL+NDSE $\leq$25)
NDSE	Total number of point detectors.

> NOTE: If (NDVOL+NDSE)=0, omit Item 20, otherwise, one card for each NDVOL detector and then one card for each NDSE detector is required.

Item 20 Detector Description (Format 3E14.6,I5,E13.6)

XAD,YAD,ZAD	The X,Y,Z coordinates of each detector. For small volume detectors, enter any point within the detector. The geometry scale factor (Item 1) does not apply; XAD,YAD,ZAD and CRAD (below) must be in centimeters.
IRDET**	(Point Detectors Only.) Region for definition of critical radius (CRAD) =-1 Critical radius (CRAD) will be read in as the next entry on this card. =0 Critical radius will be computed based on the concentration of the region in which the detector is actually located. (See footnote below) =N (N>0) Critical radius will be computed based on the concentration of region N (See footnote below)
CRAD**	(Point Detectors and IRDET=-1 Only) Enter the critical radius (cm.)

---

* All small volume regions must be lower in order than any region described with the "OR" Combinatorial Geometry operator.

** CRAD is the radius of the "critical sphere" surrounding the detector. Denoting c_i as the concentration of the "i-th" nuclide in the specified region, CRAD$\equiv(\sum_i c_i)^{-1}$. Generally use the default (blank option) for IRDET.

Item 21 Cutoff Information (Format 4E14.5)

ECUT	Low energy cutoff (ev). Tracking of a particle is terminated if its energy degrades below ECUT. However, for the thermal option (see next entry) the particle is not terminated but is restored, in energy, to ETHERM. ECUT must be greater than the lowest energy for which cross sections are available.
ETHERM	Thermal energy (ev), if a thermal group is required. For no thermal treatment, leave this entry blank. For thermal treatment, set ETHERM slightly above ECUT. IMPORTANT NOTE: NBAND must equal 0 on item 11 in order to use this option.)
FZ	Generally, $.01 \le FZ \le .10$. (See discussion Section 3.2.10). At MAGI, FZ = .05 is usually used.
EHIGH	High energy cutoff (ev). This must be less than the highest energy for which cross sections are available.

Item 22 Output Energy Bins (Format 5E14.5)*

These cards give the boundaries of the output energy bins (ev) used for the flux edit. There should be five entries per card with a total of (NOUT+1) entries. The energies should be listed from high to low. The first and last entries should be negative. Any number of negative intermediate energies may also be used, and these negative energies define the output supergroup structure (see Section 3.2.3). Note: EHIGH and ECUT must be within the output energy bins.

* The complete energy hierarchy for SAM-F is given in Appendix E.

Item 23 Output Time Bins (Format 5E14.5)

These cards give the boundaries of the output time bins. There should be five entries per card with a total of (NT+1) entries. However, if NT=0, omit Item 23 entirely. Times should be entered from high to low with the last entry equal to 0. The first entry defines TCUT, the time cutoff.

Item 24 Region Weights (Format 5E14.5)

These cards give all of the region weights needed in the problem. They are entered five to a card with a total of NRWL entries. The weights need not be entered monotonically by value but their order determines the region weight numbers (i.e., entry one is weight #1, etc.).

Item 25 Region Specifications (Format 6I5)

Use one card per region with a total of NRMAX cards. The first card applies to region 1, the second to region 2, etc.

ISC — Scoring region number in which the fluxes in this geometric region are to be stored. Several regions may be assigned the same ISC number. If ISC=0, fluxes will not be stored. There must be at least one scoring region.

NREG — Number of the composition to be found in this region.

IRW — Region weight number assigned to this region. A weight number is given by its position in the list of region weights.

IEW — Energy weight set number assigned to this region. If IEW=0, there is no energy weighting in this region.

IAN — Aiming angle number assigned to this region. If IAN=0, there is no angular weighting in this region.

IANG — Angular weight set number assigned to this region.

Item 26 Energy Weight Specification (Format 2I10)

NEWL Number of energy bins for energy weighting. ($\leq$49) If NEWL=0 there is no energy importance sampling.

NEW Number of distinct energy weight sets.

NOTE: If NEWL=0, omit Items 27 and 28

Item 27 Bin Limits for Energy Weights (Format 5E14.5)

Enter the boundaries (ev) of the energy bins to be used for energy weighting. There should be five entries per card with a total of (NEWL+1) entries. The energies should be entered in decreasing order. The lowest bin limit should be less than ECUT; the highest energy should be greater than EHIGH.

Item 28 Energy Weight Sets (Format 5E14.5)

The energy weight value in each of the above energy bins should be entered. One or more sets of energy weights may be entered. Each set should contain NEWL entries and a new card should be used to start each set. There should be a total of NEW sets. The order in which the sets are entered determines the energy weight set numbers (the first set is weight set #1, etc.).

Item 29 Angular Weight Specifications (Format 4I10)

NAIML Number of distinct aiming vectors. If NAIML=0 there is no angular importance sampling.

NUMANL Number of angular bins for angular weighting. ($\leq$49)

NUMANG Number of distinct angular weight sets.

IAIS =0 normal angular importance sampling (bias transport)
=1 bias source direction from an isotropic source (no transport biasing).

NOTE: If NAIML=0, omit items 30, 31, 32

Item 30 Aiming Directions (Format 3E14.5)

Enter the direction cosines of each aiming vector with respect to the X,Y,Z coordinates. Use a total of NAIML cards.

Item 31 Bin Limits For Angular Weights (Format 5E14.5)*

Enter the boundaries of the angular bins to be used for angular weighting. Boundaries are given in terms of the cosines of the angles with respect to the aiming vector, with the first entry equal to 1.0 and the last entry equal to -1.0. There are a total of (NUMANL+1) entries.

Item 32 Angular Weight Sets (Format 5E14.5)

The angular weight value in each of the above angular bins should be entered. One or more sets of angular weights should be entered. Each set should contain NUMANL entries and a new card should be used to start each set. These should be a total of NUMANG sets. The order in which the sets are entered determine the angular weight set numbers.

---

* If point detectors are used, there is a present restriction upon the choice of the angular weighting bin limits; the "critical volume" surrounding each point detector cannot overlap more than one angular bin.

Item 33 Source Specifications (Format 4I10)

NSR — Number of different source regions in the problem. If NSR=0, an external source or a previously generated transmission tape (tape 15) is used and no further source input is required after this card. If NSR<0, a previously generated interaction tape (TAPE 15) and a gamma ray production data tape (TAPE 12) are supplied. Skip to Item 40. For NSR<0, |NSR| is an upper limit on the number of secondary gamma rays which can be generated.

IFLAG — Number of energies used in Item 35 to define the source spectrum. If IFLAG=1, a monoenergetic source will be used. If IFLAG=0, a built-in Cranberg fission spectrum will be used for a neutron problem. (IFLAG≤150).

ISW — If ISW=0, fluxes will normalize to one source particle. If ISW=1, fluxes will be normalized to the total source power as given in the next card.

ISWW — For external source (NSR=0) only. ISWW=0 means distributed source (must be isotropic). ISWW≠0 means monodirectional source - usage is the same as for ISO, as described below in Item 34. If a transmission tape is used, ISWW is irrelevant. In case NSR<0, ISWW is automatically set =0.

NOTE: Enter Items 34-38 Only if NSR>0

Item 34 Source Regions (Formats I10,E20.10,I10)

One card is required for each source region with a total of NSR such cards

ISR* Geometrical region number

P Total power in the region (source particles per unit volume x total volume).

ISO** If ISO=0, the source will be emitted isotropically (direction may be biased, however. See Item 29).

If ISO=+1, the source will be monodirectional, with the direction specified on Item 38. No uncollided estimates are allowable for point detectors with ISO≠0.

If ISO=-1, the source will be monodirectional and the code will not try to score uncollided estimates for small-volume detectors.***

---

* Sources can be generated only in regions consisting of single bodies. The body must be a sphere, right circular cylinder, box, or rectangular parallelepiped. Also, the source regions must be lower in order than any region described with the "OR" Combinatorial Geometry operator.

** ISO must be the same for all source regions.

*** For certain geometries, involving small-volume detectors, no monodirectional uncollided rays can intercept the small-volume detectors. Setting ISO=-1, will save computer time, by instructing the code not to try to score uncollided fluxes. Under these conditions, ISO=+1 is not incorrect, it is merely inefficient.

NOTE: Omit Item 35 If Built-In Fission Spectrum Is Being Used

<u>Item 35 Spectrum Description (Format 2E20.8)</u>

These cards give the integrated source spectrum. Each card contains an energy (ev) and the integrated source above that energy, $\int_{E}^{E(1)} S(E)dE$. The first card contains the upper energy of the source with the integral equal to 0. The last card gives the lowest energy of the source with the integral equal to 1.0.* The lowest energy of the source should be less than ECUT. The highest energy of the source should be greater than EHIGH. If a monoenergetic source is desired, (IFLAG, of Item 33, =1), enter one card only with the desired value of energy in the first field and a zero (or blank) in the second field.

NOTE: Omit Items 36 and 37 For A Time-Independent Problem

<u>Item 36 Time Specifications (Format I10)</u>

NOT Number of time values used in Item 36 to specify the time distribution. If NOT=1, all radiation will be emitted at one value of time.

<u>Item 37 Time Distribution (Format 2E20.10)</u>

Each of these cards should contain a time value and the corresponding integrated source up to that time $\int_{0}^{t} S(t)dt$. The first entry should correspond to the longest time with the integral equal to 1.0. The last entry is for time equal 0 with the integral equal to 0. If all radiation is emitted at one value of time (NOT of previous item, =1) enter that value of time as the first field, and a zero (or blank) as the second item.

---

* In the present version, exponential variation is assumed between energy values. (The first cumulative integral value of 0.0 is set internally to 10^{-27}.) If exponential variation is not desired, use enough energies so that the cumulative curve approaches the same cumulative curve as for linear variation between energies.

Item 38 Monodirectional Source (Format 3E14.5)

If, on Item 34, ISO=1, the direction cosines of the monodirectional source with respect to the X,Y,Z coordinate axes should be entered. If ISO=0, omit this card. Do not use angular weighting in the source regions if a monodirectional source is specified.

> NOTE: Enter Item 39 only if ETHERM of Item 21 is >ECUT

Item 39 Thermal Neutron Diffusion Card (Formats I10,6E10.2)

This card specifies the thermal diffusion box. If the thermal cross section option is being invoked (ETHERM>ECUT) but the thermal diffusion option is not desired, leave this card blank.

ICOMP	composition number of diffusing medium
X_{min}, X_{max} Y_{min}, Y_{max} Z_{min}, Z_{max}	coordinates of the diffusing box (rectangular parallelepiped)*

* The diffusion box is currently limited to a single rectangular parallelepiped with edges parallel to the Cartesian coordinates. The box can overlap, or partially overlap, any number of regions provided they all consist of the same material composition. The diffusion box should have dimensions of at least several transport mean free paths. The input routine actually suppresses the diffusion option if any dimension is less than three transport mean free paths. Furthermore, it is recommended that the sides of the diffusion box be kept a few mean free paths from any substantial heterogeneity.

NOTE: If no volumes are to be computed, enter a blank card for Item 40.

Item 40* Volume Computation Parameters (Format 2I10,3E10.2)

NMA The number of rays to be fired for volume computation.

NST The number of rays in a statistical aggregate for the purpose of error computation.

X,Y,Z They X,Y,Z coordinates of the point from which ray are to be fired.

NOTE: If no precomputed volumes are supplied, Item 41 is a blank card. As many precomputed volumes as desired (in ascending region number) may be supplied. In any case, the last card must be blank.

Item 41* Precomputed Volumes (Formats I10,E10.3)

IP Region number of precomputed volume

VP Precomputed volume (cm^3)

Item 42 Response Function Data (Format I10)

NRESP Number of response function sets to be applied to all number flux spectra computed by the Monte Carlo game, ($-1 \leq NRESP \leq 6$).

If NRESP=0, a single response function which is always unity will be applied, and the response will be number fluxes.

If NRESP=-1, a single response function which is the average energy of the output energy bin will be applied, and the response will be energy fluxes.

If NRESP=0 or -1 Item 43 need not be applied.

* If no volume computation and no precomputed volumes are desired, then 2 blank cards corresponding to Items 40 and 41 are supplied. All volumes which are neither computed nor precomputed will be set to 1.0 by the code.

Enter the following NRESP times

Item 43 (Format 5E14.5)

R(E) The response data, in the same order as the output energy bins. Enter NOUT numbers for each set where NOUT is the number of output energy bins defined, above, in Item 17. If energy integrated fluxes are desired enter an entire response set of unity.

The response for each NRESP function sets is:

$$D = \sum_{i=1}^{NOUT} \bar{\phi}(E_i - E_{i+1})(E_i - E_{i+1})(R(E_i)).$$

3.4.2 Description of Output

The printed output consists of five parts:

1. Geometry data
2. Cross Section data
3. Monte Carlo data
4. Intermediate results
5. Results of the Monte Carlo calculation

These five parts are discussed below.

Geometry Data

The printed geometry output is basically a repeat of input data. In addition, the storage requirements in the geometry arrays are also given. As an option a printout of the internal arrays may be supplied . It is also possible to suppress all geometry data printout.

Various extra printout will be obtained if the geometry checking or picture taking options have been invoked.

Cross Section Data

The printed cross section output is basically a repeat of the input.

Each element encountered on the EDT is identified even if a particular element is not used in the problem. Thus, if an element not on the tape is specified a complete list of all elements on the tape is printed and the program will terminate.

The total length of each band is printed out and if requested, a printout of the energy banded cross section arrays will also be provided.

Monte Carlo Data

The Monte Carlo printed output data are basically a repeat of the input data.

Intermediate Results

All the parameters of the first few source particles are printed out. In number, this is the smaller of either two aggregates or 50 lines of printout. The program will also print for each statistical aggregate the following items:

Number of completed histories

Number of collisions

Number of time cutoffs and energy degrades

Number of absorptions

Number of escapes (Each estimate times particle weight)

Total energy deposition (Including by scattering and absorption events. Also, energy of particle killed by time cutoff or energy degrade is included)

Number of deaths (Including losses due to escapes, absorptions, time cutoffs and energy degrades. Each estimate times particle weight).

The number of transmissions and interactions recorded on tape 14.

Last random number sequencer (See Section 3.2.18)

Note that all but the last of the above items are cumulative. All items are printed as a single line for each aggregate.

Results of the Monte Carlo Calculation

When all the histories have been processed, a printout giving the total number of absorptions, inelastics, and transmissions will occur.

The previously discussed tallies as a function of aggregate will be repeated as a function of region. Thus, for each region the number of collisions, escapes, absorptions, etc., will be printed.

The flux and flux-functional (e.g., dose) printouts will occur next. The arrangement of the edit is as follows:

The edit is first separated into the output energy supergroups specified by the input. The supergroups are presented in order of descending energy.

Within each supergroup, the edit is next separated into time bins in order of descending time. The time limits as well as time width of each bin are printed out. Following the last time bin, results are also presented, summed over all time.

Within each time bin the results are presented first for the scoring regions and then for the detectors (point or small volume, if any).

The region (or detector) edits are presented five regions across the page and by descending energy groups down the page. Within an energy group the results are flux per ev, per second, per source particle.* (If the volume of a region was neither

* For secondary radiation transport problems the results are normalized per primary radiation particle.

preset nor internally calculated, see input Item 41, then the region and small volume detector answers must be divided by the region volume. For point detectors this is never necessary.)

For each flux answer a statistical percentage error is given. (The description of the flux and statistical percentage error calculation is given as Appendix I.) Following the last energy bin the energy-integrated results are presented for each response set. This is, for each set, the sum over all energy bins of the flux in the energy bin, times the energy width of the bin, times the appropriate value of the response function set in the bin.

3.4.3 Tape and Disk File Assignments

The following are the file (magnetic tapes or disk) assignments of SAM-F. Those assignments which correspond to the use of various options, are so labeled. File numbers refer to FORTRAN logical numbers. All files used are in the binary mode except for file 11 which is BCD mode and contains 80 column card images.

File 8 (Option)

This is used as a scratch working file when automatic banding is performed. It is also used as the sorted interaction tape for secondary gamma ray problems.

File 9

A temporary storage disk file used by the BAND subroutine. Subsequently, the file is also used for temporary storage of particle latents in the PICK routine, where it is referred to, and equivalenced to, file 18.

File 10

The organized data file (ODT). The file contains cross section data for a given problem. The structure of file 10 is given in Appendix C. File 10 may be saved for future runs.

File 11 (Option - may be omitted if File 10 from a previous run is saved.)

The element data tape (EDT). The file contains a library (SAM-X Output) of available elements. Subroutine BAND uses this tape to get the data for a given problem. BAND and its subsidiary routines are the only routines using this file. The organization of the EDT is given in Appendix A for neutrons and B for gamma rays.

File 12 (Option)

The file contains secondary gamma ray production data. (SAM-X Output).

File 13 (Option)

This file contains the organized secondary gamma ray production data. It is derived from file 12.

File 14 (Option)

The interaction/transmission file. All interactions and transmissions are written on this file for use in subsequent problems.

File 15 (Option)

An external source file. The file may also be the interaction/transmission file (File 14) from a previous run, if it is being used as a supplier of new source particles.

File 16

The statistical aggregate tape. The AMONTE routine uses this file to record each completed aggregate. The edit routines then process the file to obtain the final flux, and flux-functional results.

File 17

A temporary storage file for latents. The tape is used by the PICK routine.

File 18

See File 9.

In addition, Files 5 and 6 are the standard input and output media, respectively. File 7 has been reserved for possible future (or ad hoc) use as the standard punch medium.

3.5 Variable Core Size Requirement for the SAM-F Program

At the present time, the standard version of SAM-F loads at 120,000 - 130,000 octal locations on a CDC 6600 machine; the exact amount depending on the given computer facility. This required core allocation can be reduced or increased under certain conditions:

(1) The MASTER array holds the cross section band data as well as the output scores in the appropriate bins. The size of the MASTER array, presently 7,000, is set in the blank COMMON statement in SAMF (Main Routine). This dimensioned size is referred to as "NDQ". The user may be able to reduce this value even further. (Do not reduce NDQ below 4000.) On the other hand, the user may wish to increase NDQ to increase the output scoring bin capability (see Section 3.6) or to accommodate an unusually large bloc of gamma ray production data for a given nuclide.

Note that the number of cross section bands and thus the amount of internal tape reading and writing increases with decreasing values of NDQ. The user will have to strike his own balance. At MAGI, NDQ=7,000 to 10,000 is usually used.

(2) The FPD and MA arrays are used in the geometry routines to store body and region data, respectively. At the current dimensioned values (4000 each), about 400 bodies and regions can be treated by the code. The user may wish to reduce these arrays.

(3) Overlay AMONTE is the usually largest of the five primary overlays.* AMONTE can be reduced, and thus SAM-F reduced, under the following conditions:

(a) if no point detectors are required, it is not necessary to load ARG, ARPREP, FLUP and TRALA.

(b) if no small-volume detectors are required, it is not necessary to load FLUPV and TRALAV.

(c) if the thermal diffusion option is not required, it is not necessary to load DIFFU and DIFFUS.

(d) for primary gamma ray problems it is not necessary to load ANISOT.

3.6 Limitations Upon Size of Output Scoring Arrays

The size of the MASTER array may have to be adjusted (see Section 3.5) to accommodate desired output scoring array requirements. In addition to individual array limitations given in the Monte Carlo Input (Section 3.4.1.3), the following limitations upon NDQ must be observed:

(a) $NDQ > 2\left[(MAX)(NT)(NUMSC+NDET)\right] + NUMSC$

where MAX = maximum number of energy bins in any supergroup

NT = number of time bins

NDET = number of detectors

NUMSC = number of scoring regions

(b) $NDQ > LEGEOM + (MAX)(NT)(NUMSC+NDET) + 12NRMAX$

$+ NRWL + (NEWL)(NEW) + 3NAIML + (NUMANL)(NUMANG)$
$+ 2LFOG + 4NSR + (JSPEC)(NSR+1)$
$+ (NUMANL+1)(NSA) + 3$

where LEGEOM = storage allocated for cross sections (printed out)

NRMAX = number of regions

NEWL,NEW = number of energy importance sampling energy bins and weight sets, respectively

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* Sometimes Overlay ASORTT is the largest overlay. ASORTT can be replaced by a dummy program if a secondary gamma ray problem is not being run.

NAIML,NUMANL,NUMANG = number of angle importance sampling aiming vectors, angular bins, and weight sets, respectively

LFOG = number of energies in source spectrum

NSR = number of different source regions

JSPEC = number of energies (between EHIGH and ECUT) used to describe energy importance sampling

NSE,NSA = number of source regions which have energy and angle importance sampling, respectively.

A violation of either condition "a" or "b" will cause the code to print out a warning message and will terminate execution of the computation.

3.7 Error STOP Messages

Throughout the code various types of error conditions will cause execution to terminate. Each such stop is identified with a numbered STOP printout - often accompanied with extra diagnostic printout.

Table 3.3, below, provides the entire dictionary of SAM-F STOP messages.

TABLE 3.3

ERROR STOP MESSAGES

STOP NUMBER	ROUTINE	OVERLAY	MEANING
1	SAMF	0,0	Execution went to completion.
11	GG	0,0	ITYPE error. (ITYPE<1 or ITYPE>10)
21	G1	0,0	Region not found.
25	SEEK	0,0	Vector out of range.
31	TROPIC	0,0	Error in generating random cosine by the rejection technique.
1001	GENI	1,0	ITYPE error. (ITYPE<1 or ITYPE>10)
1003	GCHKRG	1,0	Too much data to continue geometry checking.
1011	THERM	2,0	Cumulative input data too great.
1101	AUTOBA	2,1	Too many pointers for element data.
1103	AUTOBA	2,1	Cross section upper energy is below upper energy of problem.
1105	AUTOBA	2,1	Anisotropic continuum inelastic data given. Coding not presently available to treat this option.

STOP NUMBER	ROUTINE	OVERLAY	MEANING
1107	AUTOBA	2,1	Cross section lower energy is is above lower energy of problem.
1111	AUTOBA	2,1	Elemental data is missing.
1113	AUTOBA	2,1	Index mismatch. Memory probably clobbered.
1121	CHITAB	2,1	Error in order of energies for chi-tables.
1123	CHITAB	2,1	Index mismatch. Memory probably clobbered.
1201	BAND	2,2	Too many composition elements.
1203	BAND	2,2	End of data tape reached.
1205	BAND	2,2	Element has too many pointers to be processed.
1207	BAND	2,2	Error in processing continuum inelastic scattering.
1211	BAND	2,2	Band of data is too large
1221	FILL	2,2	Error in processing energy tables.
1231	LENTHS	2,2	Index $\neq 2$ for El<EBH
1233	LENTHS	2,2	Index =1 for E>EBLX
1401	INPUTD	2,3	Negative region found for a detector.
1403	INPUTD	2,3	No room for input data.

STOP NUMBER	ROUTINE	OVERLAY	MEANING
1421	SOUCAL	2,3	IEW is negative
1423	SOUCAL	2,3	IEMP is negative
1425	SOUCAL	2,3	All EWTAB are less than EHIGH
1427	SOUCAL	2,3	ISAW(1) is negative
1431	SOUCAL	2,3	IEMP is negative
1433	SOUCAL	2,3	ISEW is negative
1435	SOUCAL	2,3	ISAW is negative
1437	SOUCAL	2,3	ISAT is negative
1441	SOUCAL	2,3	Angular importance sampling is given for an anisotropic source
1442	SOUSEC	2,3	More than 30 distinct nuclides.
1443	SOUSEC	2,3	Too many pointers in gamma ray production data set.
1444	SOUSEC	2,3	Miscellaneous reasons. See accompanying diagnostic printout.
3001	ASORTT	3,0	Too many interactions events per aggregate
4001	AMONTE	4,0	Output mesh error.
4003	AMONTE	4,0	More than 1000 statistical aggregates
4005	AMONTE	4,0	Limit of DO loop variable exceeded.
4007	AMONTE	4,0	No aggregates completed
4011	ARG	4,0	DELTL$\geq$1.0

STOP NUMBER	ROUTINE	OVERLAY	MEANING
4013	CARLO	4,0	Limit of DO loop variable exceeded.
4014	DR3	4,0	Limit of DO loop variable exceeded.
4015	FLUPV	4,0	Wrong body type for small volume estimation.
4017	FLUPV	4,0	J12345 error
4021	PICK	4,0	Various indices have forbidden values. Most likely memory has been clobbered.
4023	PICK	4,0	
4025	PICK	4,0	
4027	PICK	4,0	
4031	PICK	4,0	No room left in memory to store latent.
4033	SOUGAM	4,0	Limit of DO loop variable exceeded
4035	SOUGEN	4,0	Illegal source region.
4036	SOUPIC	4,0	Error in IR or J12 index.
4037	TRALAV	4,0	IRPRIM$\le$0

SECTION 4 - PROGRAM SAM-A

4.1 General Description of the SAM-A Program

SAM-A is an adjoint Monte Carlo code designed to calculate the response, at point or finite volume detector locations, due to fields of primary and secondary gamma radiation. The "response" may be either fluxes, or flux functionals, such as dose, heating, counting rates, etc. For the case of secondary radiation, the gamma ray sources are generated from recorded neutron interactions produced by running a precursor SAM-F primary neutron problem.

Alternatively, the code can be used to generate adjoint currents on the surface of a specified configuration (see below). These currents may subsequently be combined with available ambient radiation fields to yield the fluxes or flux functionals. In this mode, SAM-A thus operates as a "vulnerability" code.

In the Monte Carlo calculations, uncollided gamma ray contributions are made in the usual manner, i.e., by a simple $e^{-\lambda}/4\pi R^2$ type estimate, usually multiplied by appropriate weight factors. Estimates of the collided contributions, however, are made by means of an adjoint Monte Carlo game[3]. Thus the Monte Carlo histories start at the detector, time is assumed to run backwards and simulated interactions are made by use of adjoint collision mechanics. At each photon interaction point estimations of the collided contributions are made back to the source.

The gamma cross section and secondary gamma ray production data, used by SAM-A, come from ENDF and are preprocessed and made available by program SAM-X (see Section 2).

The important features of the program are described below:

(a) Use of the Combinatorial Geometry technique for description of complex three-dimensional configurations. This technique affords the user geometric capabilities exceeding those available with other commonly used geometric packages. (For secondary problems, the SAM-A program can use the same geometry input as used in the primary SAM-F neutron problem. However, the physical regions need not be numbered the same in both programs.)

(b) Primary or secondary gamma sources. The program will accept source input in the form of a neutron interaction tape (for conversion into secondary sources) or in the form of a primary gamma tape. An option also exists which allows calculation of adjoint currents at the outer surfaces of geometric regions due to Monte Carlo histories starting at a detector. These may be subsequently coupled with any number of sources in the form of time-independent gamma ray fluxes in energy and angle bins.*

(c) Time-dependent dose answers. The code keeps track of the cumulative times of flight of all photons. In addition, for secondary problems, the time of flight of the neutron is carried from the neutron problem to the adjoint gamma problem. The SAM-A program then keeps track of the total time of flight; from neutron source to gamma ray detector. Gamma ray results are calculated, in general, as functions of energy and time. However, calculation of adjoint gamma ray surface currents is presently done as a function of energy and polar angle only.

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*Refer to Appendix S for a discussion of the use of adjoint currents in calculation of doses at a detector point.

(d) Point or volume detectors.

Either a point or a volume detector may be used. In the case of a volume detector, only spheres, cylinders, rectangular parallelepipeds or boxes are presently allowed.

(e) Region and energy dependent importance sampling.

The adjoint transport and post collision energy selections are biased towards the gamma ray source, according to an input set of importance values.

A step by step description of the calculation flow is now given:

1. Read all input data (cross sections, gamma production data, geometry, importance sampling data, detector response data). If adjoint currents are desired proceed immediately to Step 4.

2. For a primary gamma ray problem read in a single source particle from the source tape and proceed to Step 4. For a secondary gamma ray problem read the neutron interaction data for a single interaction. During the previous SAM-F neutron problem all gamma ray producing interactions (absorptions and inelastics) were written on an interaction tape. For each interaction the following data was written on tape.

X(3)	neutron collision position
W(3)	direction cosines before scatter (not presently used by SAM-A because the existing coding assumes the secondary gammas are generated isotropically)*
E	neutron energy before the interaction
IR	region in which collision occured (not used by SAM-A)
T	time of flight of the neutron

* It is anticipated that this restriction will be eliminated in the near future.

ID	element identifier of interacting element
WEIGHT	neutron weight at collision point multiplied by the nonelastic interaction probability
NHIST	neutron history number
WC	carry along weight for normalization
INT	interaction indicator (INT=10)

3. Using the interaction data and the gamma production cross sections generate a secondary gamma ray. The format of the production data is given in Appendix D.

4. Select the detector position, either at a point detector or at a point within a volume distributed detector. For computation of adjoint currents proceed to Step 6.

5. Calculate the uncollided contribution from the following formula:

$$e^{-\lambda} \cdot W_{\gamma} \cdot W_{n} \cdot R(E)/4\pi r^2$$

where λ = mean free path from detector to gamma source

W_{γ} = gamma weight, set during the generation process

W_n = neutron weight at interaction

$R(E)$ = detector response at gamma source energy

r = source-detector separation distance (cm)

6. Select detector energy from detector response distribution. Select direction cosines from a distribution biased towards the gamma source. (For the adjoint current option biasing is done by means of angular weights. Section 4.3.4 describes the biasing techniques.) At this point the energy, position and direction of the adjoint gamma ray are known and the adjoint Monte Carlo game begins. At each adjoint collision point, as well as from the detector, the contribution to the collided score will be calculated.

7. Calculate the contribution to the collided score, given the gamma energy and position. (Section 4.3.8 describes the collided dose estimation technique in full detail.)

8. Select the positions for adjoint collisions along the path of the ray. As each collision point is selected, it is stored in a latent table. (If adjoint currents are computed, first score such events whose flight path intersects a surface which also bounds an escape region.) When the current ray has left the confines of the geometry a latent is retrieved. The new energy and new direction are computed and the program returns to Step 7. When all latents have been processed a new primary gamma ray or a new neutron interaction is treated. Control is transferred to Step 2.* In the near future, collision variables (position, energy, direction) will be biased so that the gamma ray weight multiplied by the collided estimate will be bounded. This biasing is described in Appendix J, but has not yet been implemented. The current code uses an approximate estimation procedure, which leads to finite variances, and which is also bounded.

9. When all neutron interactions have been processed the Monte Carlo is done and the results are edited and printed out. Items 2-8 are the basic history loop of the code.

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* Refer to Appendix K for expanded description of latents and importance sampling.

4.2 Descriptions of the SAM-A Program Input Requirements

The input requirements for SAM-A are described below. Each section discusses a different aspect of the input.

4.2.1 Cross Sections and Region Compositions

The cross section and region composition requirements are identical to those of SAM-F. As in SAM-F, the user will have at his disposal an element data tape, (EDT). This tape contains a set of energy-dependent gamma ray total cross sections. For gamma ray transport only the total cross section is required from the EDT since the scattering cross section is derived internally from the Klein-Nishina distribution.

A user must specify the material composition of each region in terms of atomic concentration (10^{24} atoms/cm^3) of each nuclide in the composition as in the formula below:

$$\text{atomic concentration} = \frac{\rho N_o}{A} \times 10^{-24}$$

where N_o = Avogadro's number = $0.6023 \cdot 10^{24}$

A = atomic weight (gms)

ρ = mass density of nuclide in the composition (gm/cm^3)

Unlike SAM-F, the SAM-A program does not "band" the gamma ray cross section data since the amount of such data, even for problems with many elements, is relatively small. Unfortunately, SAM-A also does not "band" gamma ray production data which may be relatively large.

The composition input procedure is identical to SAM-F and is given below in Section 4.4.1.

* Hopefully, this restriction will be removed in the future. An alternative approach in the mean time, is to keep "weeding" the data in SAM-X (see Section 2.4.3) until its size becomes managable.

4.2.2 Energy Mesh Specifications

The SAM-A program uses a variety of energy meshes for scoring, cross section and importance sampling purposes. The FORTRAN names for the meshes and their uses are given below. All the meshes are input to the code and are entered in monotonically decreasing order.

EGAM

The cross section energy mesh. All gamma ray total microscopic cross sections are tabulated in this mesh.

EOUT

The track length score energy mesh when a gamma ray or gamma ray production tape is specified. The track lengths through the geometry, resulting from the adjoint transport, are scored as functions of region and energy. These track lengths are edited at the end of the Monte Carlo.

ESOR

The track length score energy mesh when adjoint currents are calculated. The track lengths through the geometry, resulting from adjoint transport, are scored as functions of polar angle and energy for each region. These track lengths are edited at the end of the Monte Carlo and also written on Tape 14.

EIMP

The energy mesh for importance sampling. The importance of a region as a function of energy is tabulated in this mesh.

ENRESP

The detector results are tabulated as functions of the energy mesh "ENRESP". The initial detector energies for the transport are selected from the detector response function. All contributions to both the collided and uncollided results are scored as a function of the initial "detector" energy in the mesh ENRESP.

The five meshes discussed have a hierarchy as shown in the diagram below. Source energies must be contained in the EOUT mesh.

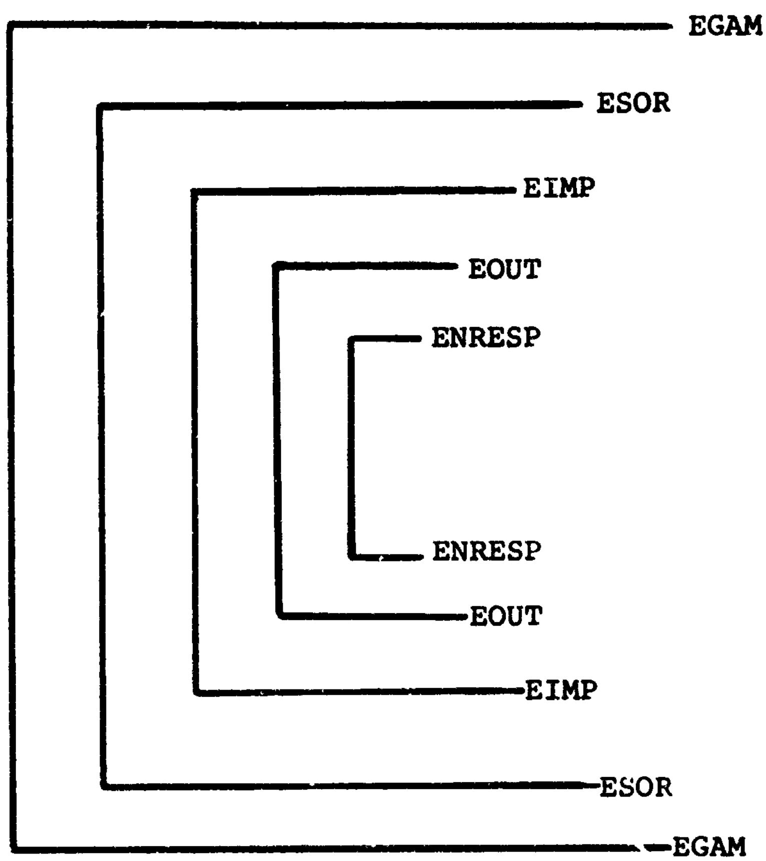


Fig. 4.1 - Energy Hierarchy in Program SAM-A

4.2.3 Source Specification

The SAM-A sources are either primary gamma rays or secondary gammas produced from precursor neutron interactions.

In the secondary gamma mode the only source input is the interaction tape and a gamma production cross section tape. The SAM-A code will convert each neutron into a corresponding secondary gamma using the production cross section data. The conversion procedure is given in the discussion of subroutine GASSUP (Section 4.3.9).

For the primary gamma mode, only an external source tape (in the same format as the interaction tape) is required unless adjoint currents are desired (in which case no source tape is utilized). The gamma source energy is used directly from the tape and no conversion is done. Section 4.4.3 describes the format of the external source tape.

4.2.4 Detector Specification

The physical detector may be either a point or a volume detector. In the case of volume detectors, the program is restricted to spheres, right circular cylinders, rectangular parallelepipeds or boxes.

The energy dependence of the detector is given in the form of an energy dependent response function from which the initial detector energies are picked. If number flux is the desired answer then the response is unity.

Note that the answers are given as functions of time and energy, (in addition to integrated results). The energy bins in which the final results are tabulated are identical to those which are used to describe the response function.

4.2.5 Output Energy Meshes

The program requires two separate energy meshes for scoring purposes. The adjoint track length answers are scored in one mesh, and detector results are scored in the other.

Note that the detector energy mesh is the same mesh used for description of the detector energy response (Section 4.2.4).

4.2.6 Time Dependence

The SAM-A program will edit detector answers as a function of time. The time bin mesh is supplied as input. For primary gamma rays, the program keeps track of the time of flight of each photon from its time of birth, to its time of arrival at the detector. For secondary gamma ray problems the "birth" time refers to that of the precursor neutron. The user must take care to provide a time bin for the longest desired time of arrival at the detector.

4.2.7 Region Dependent Parameters

For each geometric region the user must specify physical composition and the importance sampling function to be used. The physical composition is specified by "Composition number" as given in Section 4.2.1. Each region must be assigned a composition number.

The user also has the option of declaring any or all of the geometric regions as scoring regions. A "track length" edit of scoring regions is given after the completion of the Monte Carlo.* For the adjoint current option track length scores and standard deviations are also written on tape 14.

* "Track length" scores are defined as the actual path lengths (cm) of the ray through the region, multiplied by all detector response and importance sampling weighting factors.

The "scoring region" option has the additional capability of allowing the user to combine any number of geometric regions into a single scoring region for purposes of editing.

For each geometric region of the problem the user must specify an "energy weight set number". The adjoint collision mechanics and the collision density are biased according to a set of energy dependent importance numbers denoted by the "energy weight set number". Appendix K describes the importance sampling in detail.

4.2.8 Importance Sampling

The importance sampling procedure in SAM-A is the same as that used in SAM-F except for the treatment of energy selection after (adjoint) scattering. The SAM-A program selects the energy after scatter from a biased Klein-Nishina distribution. The Klein-Nishina distribution is biased according to the energy dependent weights in the collision region. These energy dependent weights are supplied as input to SAM-A. Note that a different energy dependence may be used in each geometric region.

4.2.9 Number of Histories and Statistical Groups

All answers given by SAM-A are per primary particle history, and the computed statistical errors are also given per primary particle history. For a secondary gamma ray problem the number of histories in a statistical group must be a multiple of the number used in the SAM-F neutron calculation, and the total number of histories must be less than or equal to that used in SAM-F.

4.2.10 Escape Region

The Monte Carlo game for a given gamma ray is terminated when the ray has left the confines of the geometry and entered the "escape region". The escape region must surround the entire geometry.

4.3 Additional Descriptions of the SAM-A Subroutines and Theory

The following sections will discuss the subroutines of the SAM-A program. In addition, the important analytic features of the program will be described.

4.3.1 Description of the SAM-A Program

The main program of the SAM-A gamma adjoint code controls the entire Monte Carlo calculation. The functions are outlined below:

1. Read all cross section and geometry data;
2. Read all problem parameter input;
3. Read source particles from an external tape (primary gamma ray calculations only);
4. Read neutron interactions from the Interaction tape (secondary gamma ray calculations only);
5. Make an estimate of the uncollided score via subroutine UNCOL; (this is not done for the adjoint current option)
6. Perform the adjoint gamma tracking to determine adjoint collision positions and the energy and direction of the gamma ray after an adjoint scattering event;

7. Call the secondary gamma estimation routine, ESTMT, to compute scores at the detector from each collision point (this is skipped for the adjoint current option);

8. Control all tallying and editing of all detector and track length estimates.

The basic calculation procedure is described below. The box numbers in the discussion refer to the flowchart in Figure 4.2.

Box 1

Read cross section composition data and compute $\mu_T(E)$ the macroscopic gamma ray total cross section for each composition (subroutine DATORG). For secondary photon calculations, read gamma ray production data for neutron to gamma ray conversion (GASSUP). Read geometry input data (GENI).

Box 2

All problem dependent input is read in and checked. A complete description of the input appears in Section 4.4.1.

Box 3

AGGPRO is called by SAM-A and proceeds as follows:

All answer arrays are zeroed in preparation for the Monte Carlo calculation. The program will clear the following arrays:

ANS,ANSQ,SANS	The three arrays used for storing track lengths scores and associated sums of squares for statistical error computation.
PUNC	A 900 word array used for storing collided and uncollided detector score estimates and associated sums of squares.

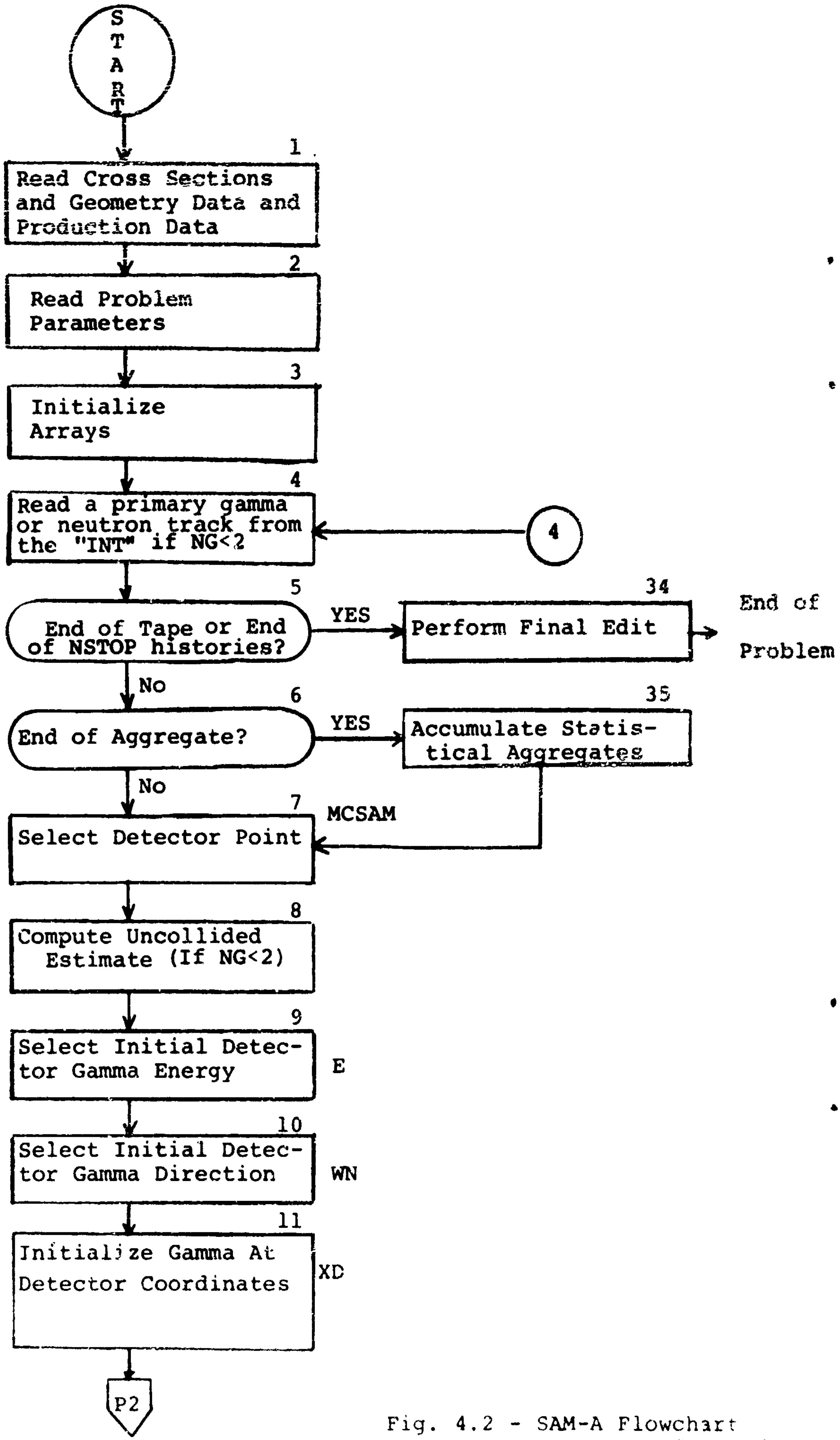
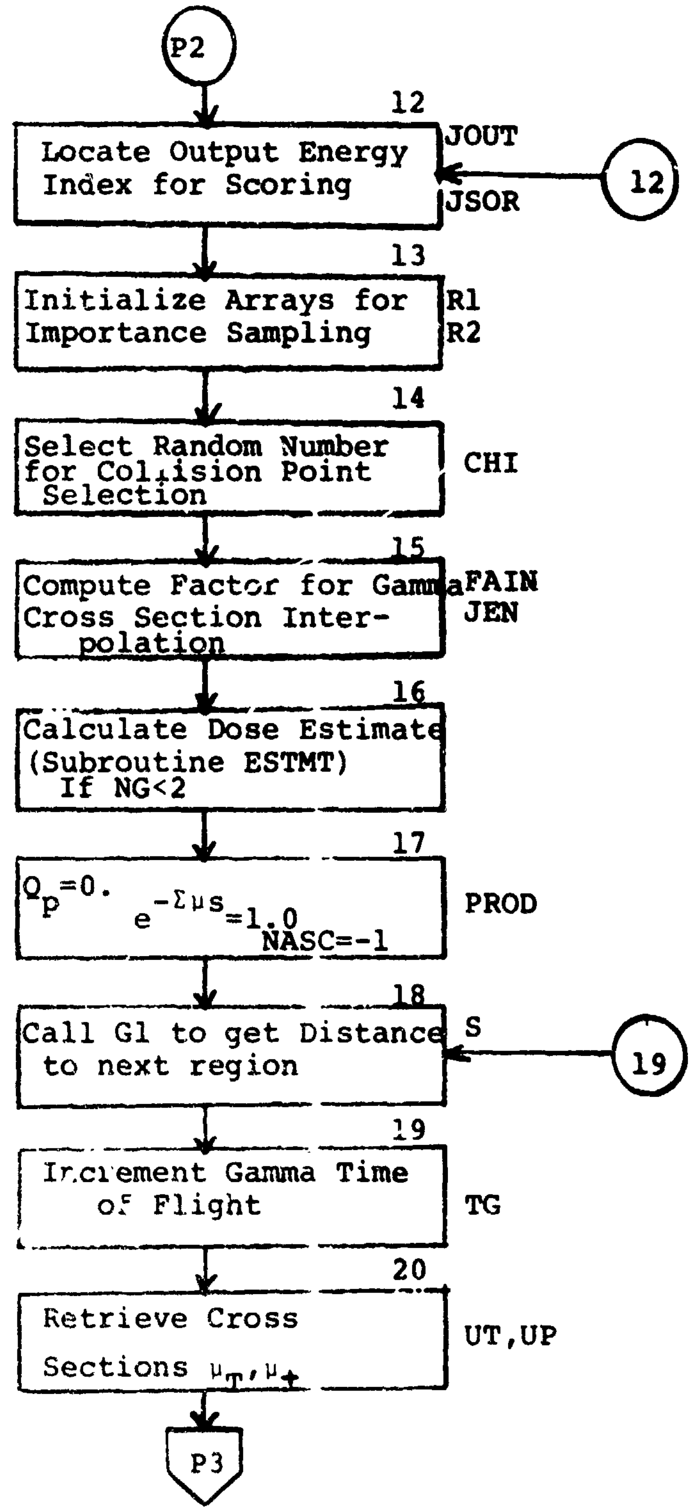
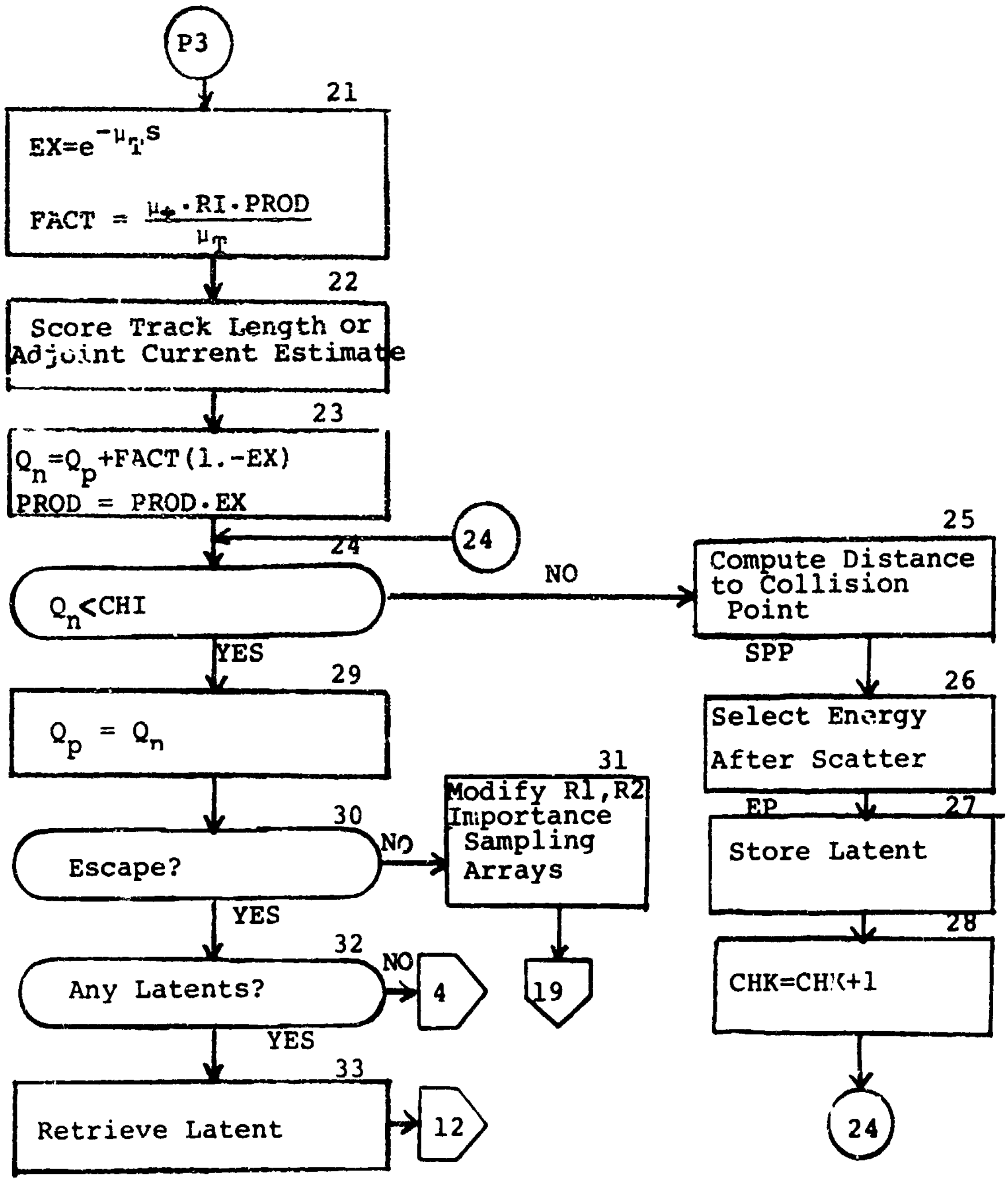


Fig. 4.2 - SAM-A Flowchart (1 of 3)



SAM-A Flowchart (2 of 3)



SAM-A Flowchart (3 of 3)

NCOL		An array giving the number of gamma collisions as a function of region and energy.

At this point all data has been read in and initialized for the Monte Carlo.

Box 4

For secondary gamma ray calculations, a neutron track is read from the interaction tape (INT) and processed for use by the gamma estimation subroutine (ESTMT). The data read from the interaction tape are described in Section 4.3.9.

For primary calculations, INT is the external source tape if NG<2.

Box 5

The parameter IR, read in from the INT tape, is normally the region number but is also used to signal the end of the tape. Specifically, if IR=0, control transfers to the final edit procedure (Box 34). If NG=2 i.e, adjoint current option, control transfers to final edit when NSTOP histories have been processed.

Box 6

The parameter NHIST (from the INT tape for NG<2) counts primary source histories and also determines when the end of a statistical aggregate has been reached. At the end of an aggregate, control is transferred to an aggregate accumulation procedure (Box 35).

Box 7

AGGPRO calls MCSAM which continues the processing. Select initial detector point according to input parameters.

Box 8

A calculation of uncollided contribution is performed. The exact procedure for the calculation is given in Section 4.3.14.

At this point all pre-collision loop data have been processed. The program will now select an initial energy from the detector distribution and a set of direction cosines from a biased distribution as computed by subroutine DIR[illegible]L.

Box 9

The initial detector energy is selected from the detector response distribution by subroutine ENDET.

Box 10

The initial direction cosines are chosen from a distribution biased towards the gamma ray source position if NG<2, or in accord with a weighted angular distribution for NG=2.

Box 11

The initial position of the gamma ray is set to the detector coordinates, XD. The initial region number is set to IRDET as supplied as input.

Box 12

All track length estimates for the current gamma ray are scored at energy E. The energy index, INPAR (INSOR, if NG=2) for the scoring array is computed here.

Note that the tracking procedure for latents and/or initial detector gammas begins here. When latents are picked up control is transferred to Box 12.

Box 13

Energy and position dependent importance sampling parameters are initialized here for use in determining adjoint collision points along the ray. The initialization consists of precomputing the integrals discussed in Appendix K.

All data are now available for the collision depositing loop which begins at Box 14.

Box 14

GRAY is called by MCSAM to continue ray processing.

An initial random number CHK, uniformly distributed between (0,1), is chosen for the stratified sampling of the collision density.

Box 15

The entire gamma track will require cross sections at the energy selected in Box 9. These cross sections are obtained by linear interpolation in the cross section array XSGAM. The linear interpolation uses a constant interpolation factor FAIN and an index JEN locating the cross section and energy in the arrays. The factor and index are computed in Box 15 and used for the current gamma track.

Box 16

The ESTMT subroutine is called to make a scoring estimate from the current gamma collision location or the detector position for NG<2. Each time a collision is made, the position, energy after scatter and associated data are stored in a latent table (see Box 27). At the end of the current track these latents are then picked up and treated as new rays Thus Box 16 will be reached for each collision and an estimate will be made.

The estimate is then scored in the array PUNL as a function of time and gamma energy at the detector.

Box 17

The initialization for the collision point selection is performed here. The collision point selection requires the recursive calculation of

$$Q_n = \sum_{i=1}^{N} \frac{\mu_{+,i}}{\mu_{T,i}} R_i \exp\left(-\sum_{j=1}^{i-1} \mu_{T,j} S_j\right)\left\{1.-\exp(-\mu_{T,i} S_i)\right\}$$

where the S_i are the track length segments for region i and the μ_+ and μ_T are the adjoint and forward total cross sections, respectively.

The initial "QP" which will be used in the calculation of "Q_n" is set to zero, and "PROD" is set to 1. The selection procedure is discussed in Appendix K.

The variable NASC which signals the start of a new ray to the geometry subroutine G1 is set to -1.

Box 18

The geometry tracking subroutine G1 is called to determine the geometric distance from the start of the ray to the next region boundary. Each call will deliver a region segment, (S), a cumulative distance, (DIST), and the region number, (IRPRIM), of the next region to be entered. Given the geometric configuration of Figure 4.3, successive calls to G1 will yield the following:

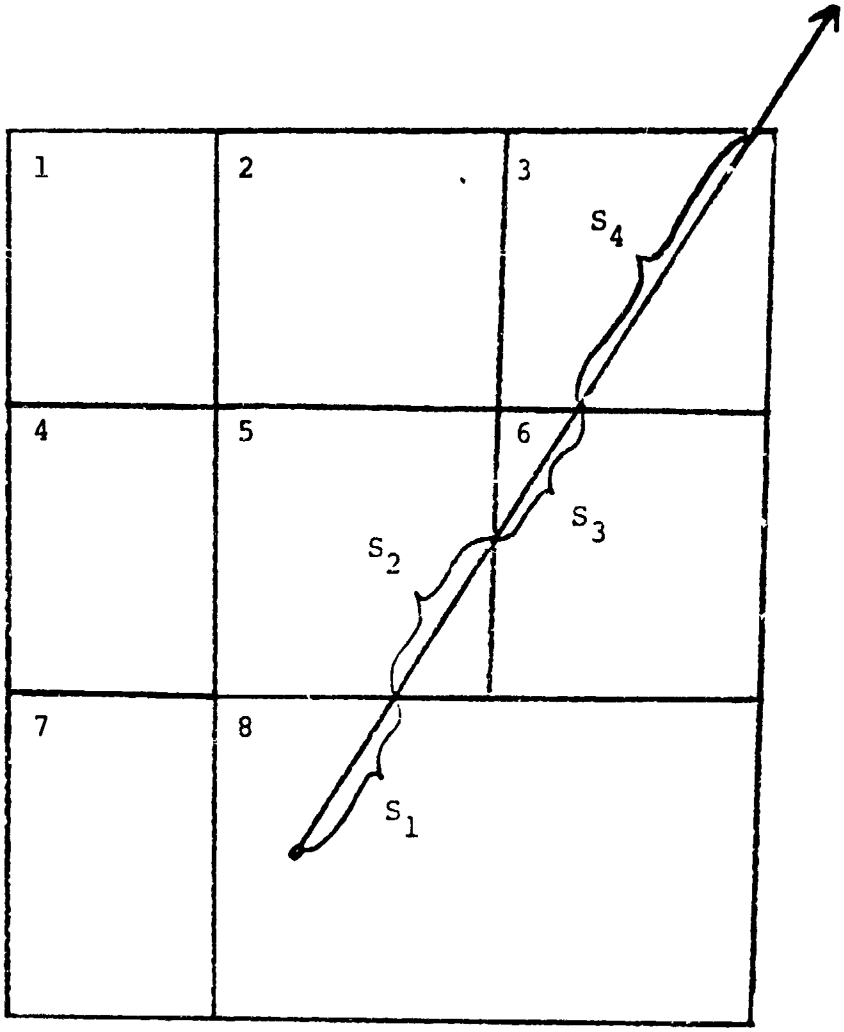


Fig. 4.3 - Geometric Tracking

(The numbers shown are region numbers.)

	S	DIST	IRPRIM
Call 1	S_1	S_1	5
Call 2	S_2	S_1+S_2	6
Call 3	S_3	$S_1+S_2+S_3$	7
Call 4	S_4	$S_1+S_2+S_3+S_4$	8

Table 4.1 - Results of Calls to Subroutine G1

Note that IRPRIM=0 when the ray leaves the confines of the geometry.

Box 19

Given the distance S through the region the time of flight TG is incremented as follows:

$$TG = TG+S*.3335637*10^{-10}$$

where the constant is the inverse of the velocity of light.

Box 21

In order to compute the Q_n from the formula in Box 17 the cross sections must be calculated. Given the interpolation factor FAIN and the energy index JEN from Box 15, the gamma ray forward total cross section μ_T is computed. The adjoint total cross section, μ_+, (UP in the program) is given as:

UP = DENSIT(IJ)*RZ/RS

where DENSIT(IJ) is the factor $\frac{3\tau\rho}{8}$

ρ is the electron density of composition IJ

τ is the Thompson unit

RS is the importance value at the current wavelength in the current region.

RZ is described in Appendix K (where it is called R_o).

Box 21

The quantities EX and PROD, used in the Q_n calculation and in the scoring of track length results are computed as follows

EX = EXP(-UT*S)

FACT = UP*RI*PROD/UT

Box 22

The track length score is now made for NG<2

ANS(INDEX) = ANS(INDEX)+PROD*S/PHIS*WEIGHT*E^2*1.9569*10^{-6}

where ANS is the scoring array for track lengths in region IR at energy E and time TG.

PHIS is the importance number at energy E at the start of the ray. WEIGHT is the carry along weight (obtained from the neutron interaction tape when applicable) which is updated when choosing the energy and direction of a new photon at the detector. For NG=2 the estimated adjoint current at the boundary with an escape region is scored. This leads to the replacement of S by EX in the formula.

Box 23

Q_n is now computed

QN = QP+FACT*(1-EX)

and the exponential factor PROD is updated

PROD = PROD*EX

Box 24

Collisions will be deposited whenever QN≥CHK, where CHK is the random number initially selected in Box 14. If a collision is to be made control will be transferred to Box 25, otherwise the next region to be entered will be examined (Box 29).

Box 25

The decision to make a collision has been made (Box 24) and the collision tally is updated

NCOL(INDEX)= NCOL(INDEX)+1

where INDEX is the location in the NCOL array of the tally for region IR and energy E.

The collision position SPP, measured from the start of the ray, is calculated from the equation of Box 18 by solving for S

SPP = DIST-S-ALOG[1+(QP-CHK)/FACT]/UT

Box 26

The energy after the adjoint scatter is calculated from the biased Klein-Nishina distribution (see Appendix L).

Box 27

A collision has been made and the position, direction before scatter, energy before and after scatter and other collision related parameters are now stored in the latent table.

The list below describes the data to be stored for subsequent processing.

X1, X2, X3	The coordinates of the collision point
W1, W2, W3	The direction cosines before scatter
WLAT	The particle weight before scatter
EL	The energy before scatter

EPL The energy after scatter

TL The time of flight to the collision point

IRL The region number of the collision point

Box 28

After the latent has been stored, the random number CHI is incremented by 1.0 and control is transferred to Box 24 to determine the next collision point along the ray.

Box 29

The collision test of Box 24 indicated no collision and a transfer to Box 29 was made to examine the next region. Thus QN replaces QP for the next computation of possible collision position.

Box 30

At this point the ray position is examined for possible escape from the geometry. If the ray escapes, control is transferred to Box 32 to process any latents created by the ray.

Box 31

The ray will now enter a new region which may have importance sampling parameters which are different from those of the previous region. If so, the importance sampling arrays established in Box 13 must be modified as described in Appendix K. After the modification control is transferred to Box 18.

Box 32,33

Control is transferred to Box 32 (from Box 30) whenever a ray has escaped the geometry. A return to MCSAM from GRAY occurs. If no latents are to be processed control is transferred to Box 4 in AGGPRO to initiate another source gamma ray and an associated adjoint gamma track.

When latents are picked up, Box 33, the cosine of the scattering angle, DEL, is calculated from the energy before and after scatter. Control is then transferred to Box 12.

Box 34 (In AGGPRO)

If the input number of histories, (or the number of histories on the INT tape), has been exceeded, control will transfer to here and the final edits will be produced. The description of output appears in Section 4.4.2.

Box 35 (In AGGPRO)

Control transfers here whenever a statistical aggregate has been completed. The aggregate accumulation arrays are updated and the array ANS that contains scores for a single aggregate is cleared. The average time per aggregate AVG and the total number of collisions thus far is printed. The computer time remaining is retrieved by subroutine STATUS. This time is compared to the average time per aggregate and the edit procedure is entered as there is insufficient time to process two more aggregates. Normally control will transfer to Box 7.

4.3.2 Description of Subroutine DATORG

Given a gamma ray element data tape (Tape 11) and the composition data as described in Section 4.2.1, the DATORG subroutine will compute total macroscopic cross section, $\mu_T(E)$ for each composition. The cross sections are stored in the XSGAM array. The atomic density for each composition is computed and stored in array DENSIT.

$$\text{atomic density} = \frac{3\tau}{8} \sum_i Z_i C_i$$

where τ is the Thompson unit

Z_i is atomic number of element i in the composition

C_i is atomic concentration of element i

4.3.3 Description of Subroutine DIREC

This routine is called by the main program to get the new direction cosines after scattering. Given an initial set of direction cosines, $\bar{\omega}$, and the cosine of the scattering angle, $\cos\theta$, the subroutine will compute a new set of direction cosines, $\bar{\omega}'$, such that

$$\bar{\omega}\cdot\bar{\omega}' = \cos\theta$$

The aximuthal angle is chosen at random.

4.3.4 Description of Subroutine DIRSEL

Subroutine DIRSEL selects the initial direction of an adjoint gamma ray, coming out of the detector in one of two ways. For NG=2 no source point is assumed and biasing is done on the basis of weights chosen in the angular bins. This is described in Section 4.3.4.2. For NG<2 the selection of the direction is done so that it is biased towards the current gamma ray source point. This improves the calculational efficiency of the code.

4.3.4.1 Implementation of the Biasing Procedure for Specified Source Points

In Figure 4.4, below, let λ_D and λ_S be the wave lengths of the photon at the detector and source, respectively:

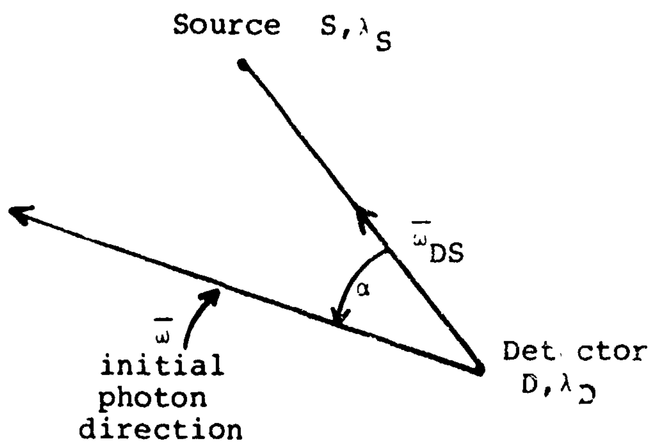


Fig. 4.4 - Geometry for Subroutine DIRSEL

The maximum possible change in λ, due to a single Compton scattering event, is given by $\Delta\lambda=2$.

In the coding, the selection of the initial photon direction is performed in two distinct modes, depending on whether $\lambda_D-\lambda_S-2$ is greater or less than zero:

a) $\lambda_D-\lambda_S-2>0$

1. The angle α is selected uniformly between 0 and π, where α is measured from the detector-to-source vector, $\bar{\omega}_{DS}$.

2. The initial direction, $\bar{\omega}$, is selected so that $\bar{\omega}\cdot\bar{\omega}_{DS}=\cos\alpha$, where the azimuthal angle is selected from an isotropic distribution.

b) $\lambda_D-\lambda_S-2<0$

1. Let $\alpha_M=$ arc $\cos(1+\lambda_S-\lambda_D)$ = maximum initial angle for single scattering estimation.

2. Divide the α domain into the intervals $(0,\alpha_M)$ and (α_M,π).

3. Choose one of the two ranges for the final selection of α. Specifically, choose the (α_M,π) range with a biased, reduced probability, p, where

$$p = \frac{\pi-\alpha_M}{(\pi-\alpha_M)+H\alpha_M}$$

and where H is an arbitrary biasing factor, (H=10 at present).

4. Select α uniformly within the chosen range.

5. The initial direction, $\overline{\omega}$, is selected so that $\overline{\omega}\cdot\overline{\omega}_{DS}=\cos\alpha$, where the azimuthal angle is selected from an isotropic distribution.

It is straightforward to show that the following weight adjustments are made for the above-mentioned process for selecting the initial photon direction:

Selection Mode	Weight Adjustment Factor
$\lambda_D-\lambda_S-2>0$	$(\pi/2)\sin\alpha$
$\lambda_D-\lambda_S-2\leq 0$	
a) $\alpha<\alpha_M$	$\left[\frac{(\pi-\alpha_M)+H\alpha_M}{H}\right]\frac{\sin\alpha}{2}$
b) $\alpha\geq\alpha_M$	$\left[(\pi-\alpha_M+H\alpha_M)\right]\frac{\sin\alpha}{2}$

Table 4.2 - Selection Modes for Initial Photon Direction

4.3.4.2 Implementation of the Biasing Procedure for Unspecified Source Points

The choice of the direction imparted to a ray starting at the detector is done on the basis of a biased angular distribution. An input biasing axis is chosen on input. A set of polar cosines about the biasing axis is also specified. The direction of a ray is then determined on the basis of a biased density distribution that is read in as input and the proper weighting of the history is maintained.

4.3.5 Description of Subroutine DOSEDT

The DOSEDT routine prints the detector responses (i.e., flux, dose, etc.) as functions of energy and time using the energy mesh of the detector response. The routine is called, from the main program, once for each time bin and also for the time integrated results. For each time bin, the collided, uncollided and total results, as functions of energy, are printed out with associated deviations. The energy integrated results are also printed out.

Note that all answers are normalized to one primary particle history and are also divided by the appropriate value of Δt and ΔE. Thus the results are on a per primary source particle per unit time (sec) and per unit energy (ev) basis.

4.3.6 Description of Subroutine EDIT

The EDIT subroutine prints the track length scores if NG< 2 (or the adjoint current scores for NG=2) and associated deviations as functions of energy and region (cosine). The energy mesh used is EOUT (or ESOR) as described in Section 4.2.5. All answers are normalized to one primary source particle and divided by the appropriate value of ΔE. This subroutine is the same as that used in SAM-F except that no additional response function calculation is provided, since the detector particle energies are selected directly from the normalized response function.

4.3.7 Description of Subroutine ENDET

This routine is called from the main program to select the initial detector energy. The initial energy is chosen from the detector response function supplied as input.

4.3.8 Description of Subroutine ESTMT

In SAM-A, the uncollided contributions to the detector score are made analytically each time a new photon history is begun. Contributions to the collided component of the score are made by subroutine ESTMT.

The once-collided estimate is made from the detector position by first selecting an "appropriate" intermediate point (see below) and then by scoring for the detector-intermediate point-source geometry. This is shown in Figure 4.5, below. Further collided estimates are subsequently made after each adjoint Monte Carlo collision, again by first selecting an "appropriate" intermediate point for the estimation process.

The reason for the use of an "intermediate point" in the estimation process has to do with the nature of photon sources. The energy spectra of these sources, particularly for secondary gamma rays, consist partly (or completely) of discrete energy lines. Obviously, the energy of an adjoint photon which is aimed at the source point from the current collision point, cannot be exactly the same as the energy value of one of these lines. Hence collision point-to-source hookups would be impossible in the adjoint game.

SAM-A overcomes this difficulty by judiciously selecting an intermediate point (point I, in Figure 4.5), such that the energy of the photon heading from I towards the source does indeed match the energy of one of the discrete lines.

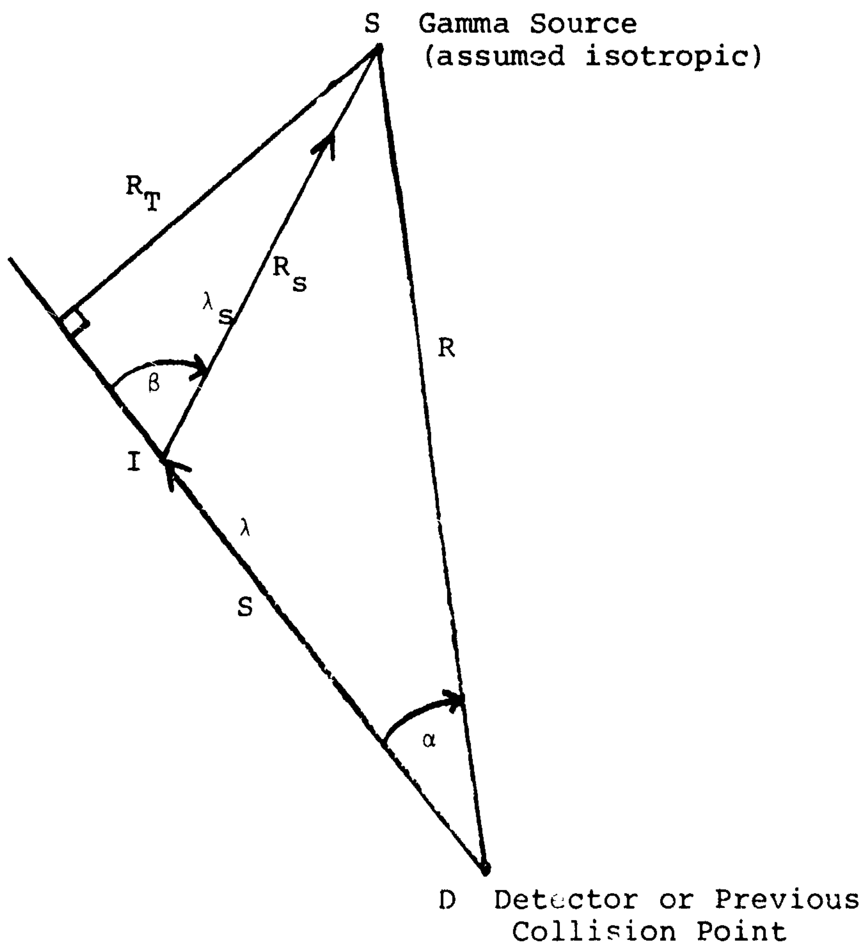


Fig. 4.5 - Collided Estimation Geometry
(arrows denote adjoint game path)

In Figure 4.5 let λ_S be the wavelength of the photon coming out of collision at I, and let λ be the wavelength of the photon coming out of the adjoint collision at D. (For the once-collided estimate, D represents the detector point.)

Then the estimate, B, of the collided contribution is given by:

$$B = W \times k(\lambda_S,\lambda) \int_0^{\infty} \frac{e^{-\int_0^{R_S} \mu(\lambda_S)dr}}{4\pi R_S^2} \times e^{-\int_0^{S} \mu(\lambda)dr} \times \delta(\lambda_S-(\lambda-1+\cos\beta))dS \tag{48}$$

where $k(\lambda_S,\lambda)$ is the forward mode Klein-Nishina Kernel corresponding to a change in wavelength from λ_S to λ,

μ is the total cross section,

and W is a weight adjustment factor which contains several components. Discussion of W is reserved for the end of this section.

In expression 48, let $\Delta = \cos\beta$, then the δ-function can be eliminated to give:

$$B = W \times k(\lambda_S,\lambda) \left|\frac{dS}{d\Delta}\right| \frac{\exp\left[-\int_0^{S}\mu(\lambda)dr - \int_0^{R_S}\mu(\lambda_S)dr\right]}{4\pi R_S^2}$$

when S and $|\frac{dS}{d\Delta}|$ are determined from the value of Δ given by $\Delta = \lambda_S - \lambda + 1$. A simple geometric derivation, (see Figure 4.5), gives:

$$S = (\cos\alpha - \frac{\cos\beta\sin\alpha}{\sin\beta})R$$

from which $|\frac{dS}{d\Delta}|$ can be derived.

$$|\frac{dS}{d\Delta}| = |\frac{\sin\alpha}{\sin^3\beta}|R$$

Since $R_S\sin\beta = R_T = R\sin\alpha$,

$$\frac{1}{R_S^2}|\frac{dS}{d\Delta}| = \frac{1}{R_T|\sin\beta|}$$

As a result

$$B = W \times \left[\frac{k(\lambda_S,\lambda)}{4\pi R_T|\sin\beta|}\right]\exp\left[-\int_0^S \mu(\lambda)dr - \int_0^{R_S} \mu(\lambda_S)dr\right]$$

This estimator is not bounded due to the presence of the $R_T\sin\beta$ term in the denominator. A biasing technique has been developed, although not yet implemented, to obtain a bounded estimator. This is described in Appendix J.

In order to avoid an unbounded estimate, until the technique of Appendix J is implemented, SAM-A makes use of an "**approximate** bound" estimator. Specifically, if $R_T < R_O$, the term $1/R_T$ is replaced by $2/R_O$ for estimation purposes. R_O is defined as the minimum of the distance equivalent to 0.1 mean free paths, measured at the source gamma energy, and the distance between the gamma position and the source position.

If $|\cos\beta| > .99$, the $1/\sin\beta$ term is replaced by a constant, 14.1539473325, which is the calculated value of $\beta_O/(1-\cos\beta_O)$, where $\beta_O = \text{arc}\cos(.99)$.

The first term, in the estimation expression, is W, the weight factor. This is a composite of several terms which are now discussed.

The energy, E, of the photon from the detector is selected from the response function, R(E), in the energy range E_S to E_L - where E_S is selected gamma ray source energy and E_L is the cutoff energy of the problem.

Since the adjoint scattering mechanics are carried out on a wavelength basis (i.e., not in energy) a weight adjustment $= |d\lambda/dE|$ is necessary:

$$\lambda = \frac{.511}{E} \quad , \text{ E is in Mev}$$

$$\therefore \left|\frac{d\lambda}{dE}\right| = \frac{.511}{E^2}$$

The total weight adjustment, necessitated by the selection of energy E at the detector is then seen to be:

$$\frac{.511}{E^2} \times \int_{E_L}^{E_S} R(E)\,dE$$

Finally, the weight term W includes all the additional weight factors due to prior games of importance sampling played by the photon and, for secondary problems, by the precursor neutron.

4.3.9 Description of Subroutine GASSUP

The GASSUP subroutine is called by the main program to convert neutron interactions into secondary gamma ray sources. The conversion process is described below.

During the previous SAM-F neutron problem all interactions were written on an interaction tape. For each interaction the following data was written on tape.

X(3)	neutron collision position
W(3)	direction cosines before scatter (not presently used by SAM-A because the existing coding assumes secondary gammas are generated isotropically)
E	energy before scatter
IR	region in which collision occurred (not used by SAM-A)
T	time of flight of the neutron

ID	element identifier of interacting element
WEIGHT	neutron weight at collision point x nonelastic scattering probability
NHIST	neutron history number
WC	carry along weight for normalization
INT	The variable INT is set to "10" indicating an interaction.

Using the interaction data and the gamma production cross sections, GASSUP generates a secondary gamma ray. The production data is given as a separate matrix for each element. For each matrix the gamma production multiplicity is given as a function of neutron energy bin and gamma energy line. Thus, for an interaction at a specified neutron energy, a gamma energy is selected from the distribution of gamma lines in the corresponding neutron bin. A gamma weight, which is the sum of all multiplicities for the neutron bin x the precursor (neutron weight), is calculated. This gamma ray weight is carried along and used in the subsequent adjoint Monte Carlo game.

The GASSUP program is called at the beginning of the main program to read the gamma production data from tape 7. The format of the data is given in Appendix D. All subsequent calls to GASSUP convert the next neutron interaction into a secondary gamma ray.

4.3.10 Description of Subroutine POSGEN

The POSGEN routine selects uniformly distributed points within the detector volume. The routine is called from the main program at the start of each gamma ray history. The selection procedure for the allowed body types is as follows. In all cases, ξ represents a random number selected from a uniform distribution from 0. to 1.

SPHERE

$$r = \mathrm{MAX}(\xi_1, \xi_2, \xi_3) R^*$$

$$\bar{X} = \bar{X}_o + \bar{\omega} \cdot r$$

where $\bar{X}_o$ = center of sphere

$\bar{\omega}$ = cosines selected from an isotropic distribution

R = radius of sphere

RIGHT CIRCULAR CYLINDER

$$\bar{X} = \bar{V} + \bar{H} \cdot \xi_1 + \bar{\omega} \cdot \mathrm{MAX}(\xi_2, \xi_3) \cdot R^*$$

where $\bar{V}$ = vertex of cylinder

$\bar{H}$ = height vector

R = radius

$\bar{\omega}$ = direction cosines selected isotropically in the plane normal to $\bar{H}$

BOX

$$\bar{X} = \bar{V} + \xi_1 \bar{H}_1 + \xi_2 \bar{H}_2 + \xi_3 \bar{H}_3$$

where $\bar{V}$ = vertex of box

$\left.\begin{matrix} \bar{H}_1 \\ \bar{H}_2 \\ \bar{H}_3 \end{matrix}\right\}$ = height vectors of box

RECTANGULAR PARALLELEPIPED

$$X = X_L + \xi_1 \cdot (X_U - X_L)$$

$$Y = Y_L + \xi_2 \cdot (Y_U - Y_L)$$

$$Z = Z_L + \xi_3 \cdot (Z_U - Z_L)$$

* $X = \mathrm{MAX}(\xi_1, \xi_2, \ldots, \xi_N)$ samples X from a probability distribution function proportional to x^{N-1}.

where the X_L, X_U, Y_L, Y_U, Z_L, Z_U are the three sets of "upper" and "lower" bounding planes of the parallelepiped.

4.3.11 Description of Function RANF

The RANF function generates uniformly distributed random numbers on the range (0,1). Each use of RANF gives a different random number. The same generator is used in SAM-F.

4.3.12 Description of Subroutine SET

The SET subroutine is called from the main program to initialize arrays for the Monte Carlo calculation. A call to SET,

CALL SET(A,N,ARG)

will initialize "N" values of array "A" to the value "ARG".

4.3.13 Description of Subroutine SEEK*

Each call to SEEK,

CALL SEEK (X,A,N,I)

will perform a binary search in the array "A" of length "NOUT+1". and return the value "I" such that

$A(I) \geq X > A(I+1)$ for A monotonically decreasing

$A(I) < X \leq A(I+1)$ for A monotonically increasing

The value "I" is set to "0" for "E" outside the range "A".

4.3.14 Description of Subroutine UNCOL

The UNCOL subroutine calculates the uncollided response contribution to the detector from a gamma source of energy E_γ. The uncollided score is given by

$$S(E,r) = e^{-\lambda} \cdot W \cdot R(E_\gamma)/(4\pi r^2)$$

* This is not identical to the SEEK routine in SAM-F.

where λ is the mean free path distance from source to detector

W is the appropriate weight factor

$R(E_\gamma)$ is detector response at E

r is the distance from source to detector

4.3.15 Description of Combinatorial Geometry Subroutines

The Combinatorial Geometry package consists of the following subroutines:*

GARB	arbitrary polyhedron input processor
GENI	geometry input processor
GG	distance calculating routine
GGTEC	distance calculating routine for truncated elliptical cones
G1	main ray tracing routine
GP	debug printout routine
GETIR	determines the region of a given point

The package was discussed previously in the SAM-F section of this report, (Section 3).

4.4 Input, Output and Tape Assignments

The following sections describe the card input forms for SAM-A, the general form of the output edits, and the tape/disk requirements of the program.

4.4.1 Card Input Formats

The card input formats are given below in the order in which they are to appear in the data deck.

Item 1 - Cross Section Composition Identification (Format 2I10)

NCOMP - total number of compositions in the problem (≤ 12)

IPR = 0, no cross section edit

= 1, print total cross sections for each composition

Repeat Items 2 and 3 for each (NCOMP) composition.

*The Geometry Checker routines also may be added to SAM-A.

Item 2 - Number of Elements (Format I10)

NE - number of nuclides in present composition

Repeat Item 3 for each (NE) nuclide in present composition.

Item 3 - Element Card (Format 10X,I10,E15.6)

ID - an integer which identifies the nuclide (5 decimal digits ZZAAA)

ZZ = atomic number

AAA = truncated atomic weight for a nuclide

= 000 for a naturally occurring mixture of isotopes

CONC - atomic concentration of nuclide in this composition in units of 10^{24} atoms/cm^3.*

Item 4 - Geometry Input

This section is the same as that used by SAM-F and is described in Section 3.4.1.1 (Items 1-10).

Item 5 - General Parameters (Format 3I10,9I5)

NSTART = Maximum running time in seconds **

NSTOP = Total number of primary particle histories ***

NSTAT = Number of primary histories per statistical group

NRMAX = Number of geometric regions (≤ 200)

NG = 0, neutron interaction tape supplied for source

= 1, external gamma ray source tape supplied

= 2, score (time-independent) currents leaving the scoring regions

* Calculate by multiplying weight density in material (grams/cm^3) by $\frac{.6023}{A}$ where A = non-truncated atomic weight (gms) and .6023 is Avogadro's Number times 10^{24}.

** Upon completion of each statistical aggregate the code estimates the total (real) running time at the end of two additional aggregates. If this time exceeds NSTART (seconds) no new aggregates will be started and control is switched to the edit routines.

*** Refers to primary neutron histories for secondary gamma ray problems.

Item 5 - Continued

MT = Number of time bins ($\leq$25); for no time dependence us MT=0 (No time dependence is currently allowed for NG=2 option)

NOUT = Number of output energy bins ($\leq$25) (Set NOUT=1 for NG=2 option)

MRS = Number of scoring regions

NRWL = Number of distinct regions weights ($\leq$100)

IBG = 0, no debug printout

= 1, debug printout

MUL = Number of times each neutron interaction is to be used (if a zero is entered, the code assumes MUL=1)

Item 6 - Detector Parameters (Format 3E14.6,I4)

XD = Detector coordinates (x,y,z); (for point detector only)

IRDET = Detector region number* (use negative number for point detector, or a positive number for volume detector)

Item 7 - Output Gamma Energy Mesh (Format 5E14.5)

The mesh at which the track length scores will be tallied. Enter NOUT+1 numbers from high to low energy. Use as many cards as required.

Item 8 - Output Time Bin Mesh (Format 5E14.5)

Time mesh (seconds) at which detector scores will be tallied. Enter MT+1 numbers from longest to shortest times. Omit this set if MT=0.

Item 9 - Region Weights (Format 5E14.6)

Enter the NRWL region weights to be used in the problem. The weights need not be entered monotonically by value but their order determines the region weight numbers (i.e., entry one is weight #1, etc.)

*The volume detector must be a region restricted to a single body. Either a sphere, right circular cylinder, box, or rectangular parallelepiped is allowed. Furthermore, no regions employing the (OR) operator, see Section 3.2.1.1, may sequentially preceed this detector region.

Item 10 - Region Parameter Data (Format 4I5)

ISC = Scoring region number. (For NG=2, ISC is scoring region at whose common boundary with the escape region currents all scored).

ICMP = Physical composition number

IRW = Region weight number

ISN = Energy importance set number

Enter one card for each geometric region, a total of NRMAX cards.

Item 11 - Importance Sampling Parameters (Format 2I10)

NEI = Number of bins in the energy importance mesh (≤ 24)

NSET = Number of importance sets

Item 12 - Energy Mesh for Importance Sampling (Format 5E14.5)

Enter NEI+1 numbers from high to low energy (ev).

Item 13 - Importance Sampling Numbers (Format 5E14.5)

Enter each set of importance numbers (NSET numbers) in same order as the energy mesh for importance sampling. Each set starts a new card.

Item 14 - Response Function Length (Format I10)

NBRESP = Number of energy bins for the response function from which the "detector" photons are selected.

Item 15 - Energy Mesh for Response Function (Format 5E14.5)

Enter NBRESP+1 numbers from high to low energy (ev).

Item 16 - Response Function Values (Format 5E14.5)

Enter NBRESP values of the response function corresponding to the energy bins defined in Item 14. (If flux is the desired response enter all values at 1.0.)

> **NOTE:** Enter Items 17-24 only if NG=2 (See Item 5)

<u>Item 17 Scoring Parameters (Format I10)</u>

MWSR - Number of polar angle cosine bins ≤ 34

MSOR - Number of scoring energy bins ≤ 34

<u>Item 18 Scoring Polar Angle Cosines (5E14.5)</u>

Polar cosine mesh. Enter MWSR+1 cosines, in descending order, from +1. to -1.

<u>Item 19 Scoring Energies (5E14.5)</u>

Scoring energy mesh (ev). Enter MSOR+1 numbers, in descending order.

<u>Item 20 Scoring Axis Direction Cosines (3E14.5)</u>

Specification of direction cosines of the axis for polar cosine mesh as specified in Item 18. Enter x,y,z direction cosines in order.

<u>Item 21 Biasing Axis Direction Cosines (3E14.5)</u>

Specification of aiming axis about which is specified a polar cosine mesh for biased selection of the direction out of the detector (Item 23). Enter x,y,z direction cosines in order.

<u>Item 22 Number of Biasing Polar Cosine Bins (I10)</u>

Enter number, NB, of such bins. ≤ 20

<u>Item 23 Biasing Polar Cosine Mesh Points (5E14.6)</u>

Enter NB+1 cosines, in descending order, from +1. to -1.

<u>Item 24 Biasing Polar Cosine Direction Weights (5E14.6)</u>

Enter NB weights.

<u>4.4.2 Description of Output</u>

The SAM-A output falls into the following general categories (in the order in which they are printed).

a. Cross section and composition information,

b. Geometry information,

c. Problem input data,

d. End of aggregate tally,

e. Track length or adjoint current scores,

f. Gamma ray collision tally,

g. Detector edit. (NG<2)

The following sections describe each of the above categories:

a. Cross Section and Composition Information

The printed cross section output is basically a repeat of the input.

Each element encountered on the element data tape, (EDT), is identified even if a particular element is not used in a problem. Thus, if an element not on the EDT is specified a complete list of all elements will be printed and the program will terminate.

b. Geometry Data

The printed geometry data is basically a repeat of input data. In addition, the storage requirements for the geometry arrays are given. As an option, a printout of the internal geometry arrays may also be given. As an additional option, all geometry printout may be suppressed.

c. Remaining Input Data

The remaining problem input data are printed out.

d. End of Aggregate Data

At the end of each aggregate a one line summary for that aggregate is given. Eight numbers are printed acorss the page.

(1) Final history number for the aggregate.

(2) Average time per history.

(3) Average time for the aggregate.

(4) Cumulative number of adjoint collisions.

(5) Total response at the detector.

(6) Percentage error in the total response.

(7) Cumulative number of collided estimates resulting in in non-zero estimations.

(8) Cumulative number of gamma sources created and used for tracking.

After the final aggregate the total Monte Carlo running time is printed.

e. Track Length or Adjoint Current Scores

If NG<2 for each region designated as a scoring region, (input parameter), the track length scores as functions of the track length energy mesh (also input) will be printed. The displayed results have been divided by ΔE and by the number of primary histories. This edit is time-integrated and is, in general, the same as used for track length scores in the SAM-F program. Note that the answers are not divided by the region volumes.

In addition to the energy dependent scores, the energy integrated scores are also given for each region.

If NG=2, the adjoint currents are printed rather than the track length scores. For each scoring region they are given as a function of the adjoint current energy and polar cosine meshes.

f. Gamma Ray Collision Edit

The number of gamma ray collisions in each geometric region, (as a function of energy, using the track length energy mesh), is printed. Region numbers are given across the page and energy bin bounds are given down the page.

g. Detector Response Edit

The detector response edit gives the uncollided, collided and total detector responses as functions of energy and time. The results are scored in bins using the energy mesh for the response function data and the input-specified time mesh. The units of the response correspond to the detector response function supplied as input. Hence, if the input response function was flux-to-dose conversion factors, the final results are doses. If a unity response function was supplied, the results are number fluxes. If the average energy of a scoring energy bin was enetered, the results are energy fluxes, etc.

Each time bin is edited separately and the energy integrated response is given for each time bin. In addition, a time-integrated response is given after the time-dependent results for each time bin have been printed.

4.4.3 Tape and Disk File Assignments

The following are the file (magnetic tapes or disk) assignments of SAM-A. File numbers refer to FORTRAN logical numbers.

File 7 (Option)

The gamma ray production cross section file.

File 11

The gamma ray cross section tape.

File 14

If NG<2 it is the neutron interaction tape or the primary gamma source tape. When NG=2 the adjoint currents are written on tape in the form of BCD records.

In addition, Files 5 and 6 are the standard input and output media, respectively.

When NG=2 the interactions or gamma ray sources are written on the tape in blocks of 35 particles per record with the following write statement

```
WRITE(14) ((B(I,J),I=1,14),J=1,35)
```

Thus each column of "B" is a 14 word particle record.

The format of each 14 word particle record on File 14 is shown below.

Word	Interaction Tape	Primary Gamma Tape
XB(3)	Neutron Collision Position	Gamma Ray Source Position
WB(3)	Direction Cosines before neutron collision	Direction Cosines from isotropic distribution
E	Neutron energy before collision	Gamma Ray Source energy
IR	Region of neutron collision	Not used
T	Time of flight to collision	Arbitrary starting time for gamma ray
IDET	Identifier of interacting element	Not used
F	Neutron Weight	Arbitrary Weight which will multiply all scores
NHIST	History number	History number
WC	Weight factor computed by SAM-F	Must be "1.0"
J12345	Must be "10"	Must be "1"

TABLE 4.3 - FILE 14 FORMAT

Note that the last record on the tape must have all zeroes except for the history number which must be the last history on the tape plus one.

For NG=2, the following is written on tape 14:

Item 1: NRSOR (I10). NRSOR is the number of scoring surfaces.

The following are written NRSOR times.

Item 2: NWSR, NSOR (2I10). NWSR, NSOR are the number of mesh cosines and energy, respectively.

Item 3: (WSOR(I),I = 1,NWSR) (5E14.5). WSOR(I) are the mesh cosines.

Item 4: (ESOR(I),I = 1, NSOR) (5E14.5). ESOR(I) are the mesh energies.

The following are written as an energy-cosine matrix with an inner cosine loop of dimension MWSR=NWSR-1 and an outer energy loop of dimension MSOR=NSOR-1.

Item 5: FLUX(I), SD(I). FLUX(I) are the adjoint currents and SD(I) are their percent standard deviations.

SECTION 5 - REFERENCES

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APPENDIX A

Organization of the Neutron Element Data Tape (NEDT)

The neutron element data tape is created, one element at a time, by program SAM-X. Each elemental set of data on the EDT is written as a series of logical binary records, each 510 words long. The number of such records for an element is given, in fixed point arithmetic, by:

$$\frac{(\text{NLENTH}-1)}{510} + 1$$

where NLENTH is the number of words of data for the element (see "1st word" below).

The elemental data arrays consist of energy tables, cross section data and series of pointers and word length indices. The pointers and indices and the organization of the data array were carefully designed so as both to eliminate unnecessary data (e.g., inelastic scattering cross sections equal to zero) and to maximize the efficiency of the cross section lookup.

The following is a description and a map of the organization and contents of the EDT for one element. This is followed by an organizational chart.

LOCATION	CONTENTS	COMMENTS
1st word	NLENTH	NLENTH=number of words of data for this element;
2nd word	ATWT	ATWT=atomic weight;
3rd word	ID	ID=the ENDF (ZZAAA) designation for the material (not the MAT #);

Preceding page blank

LOCATION	CONTENTS	COMMENTS
4th word	IT	IT is currently ignored;
5th word	LCETAB	LCETAB=pointer* for the basic energy table;
6th word	LOCT	LOCT=pointer for the total cross section table
7th word	LOCS	LOCS=pointer for the total scattering cross section table;
8th word	LOCI	LOCI=pointer for the total inelastic cross section table;
9th word	LOCM	LOCM=pointer for the table of multiplicities;
10th word	NEN	NEN=number of words (energies) in the basic energy tables;
11th word	NI	NI=number of words in the total inelastic cross section table;
12th word	NM	NM=number of words in the multiplicity table;
13th word	LOCEK	LOCEK=pointer for elastic chi information (elastic T-table);
14th word	LOCLEV	LOCLEV=pointer for discrete level information;
15th word	LOCCON	LOCCON=pointer for continuum inelastic information;
16th word	LOCEXT	LOCEXT is currently ignored;
(Start of Elastic T-Table)		
LOCEK-1	NMXEK	NMXEK=maximum number of chis (χ) for an elastic chi table;
LOCEK	LCENEK	LCENEK=pointer for elastic chi energy table:

* See remark #8 for explanation.

LOCATION	CONTENTS	COMMENTS
*LOCEK+1	LOCEK1	LOCEK1=pointer for the elastic χ_1 table;
.	.	
.	.	
*LOCEK+NMXEK	LOCEKN	LOCEKN=pointer for the elastic χ_{NMXEK} table;
LOCEK+NMXEK+1	NENEK	NENEK=number of energies in the elastic chi energy table;
LOCEK+NMXEK+2	NEK1	NEK1=number of entries in the elastic χ_1 table;
.	.	
.	.	
LOCEK+2*NMXEK+1	NEKN	NEKN=number of entries in the elastic χ_{NMXEK} table;
(end of elastic T-table)		
LOCLEV-1	NLEV	NLEV=number of discrete levels;
LOCLEV	NLEVHI	NLEVHI=number of high energies in basic table not having a corresponding level cross section entry;
LOCLEV+1	LOCL1	LOCL1=pointer for level 1 cross section entries;
.	.	
.	.	
LOCLEV+NLEV	LOCLN	LOCLN=pointer for sum of all NLEV level cross section entries;
LOCLEV+NLEV+1	NL1	NL1=number of entries in level 1 cross section table;
.	.	
.	.	
LOCLEV+2*NLEV	NLN	NLN=number of entries in the sum through level NLEV cross section table;
LOCLEV+2*NLEV+1	ENL1	ENL1=excitation energy for level 1;
.	.	
LOCLEV+3*NLEV	ENLN	ENLN=excitation energy for level NLEV;
LOCLEV+3*NLEV+1	LOCKL1	LOCKL1=pointer for level 1 T-table (analogous to LOCEK for elastic T-table)
.	.	
.	.	
LOCLEV+4*NLEV	LOCKLN	LOCKLN=pointer for level NLEV T-table;
(Start Level 1 T-Table)		
LOCKL1-1	NMXL1K	NMXL1K= maximum number of chis for a level 1 chi table;

---

* Whenever entries are separated by dots, the existence of the necessary intermediate entries is implied.

LOCATION	CONTENTS	COMMENTS
LOCKL1	LCEL1K	LCEL1K=pointer for level 1 chi energy table;
LOCKL1+1	LCL1K1	LCL1K1=pointer for the level 1 χ_1-table;
⋮	⋮	
LOCKL1+NMXL1K	LCL1KN	LCL1KN=pointer for the level 1 χ_{NMXL1K}-table;
LOCKL1+NMXL1K+1	NENL1K	NENL1K=number of energies in the level 1 chi energy table;
LOCKL1+NMXL1K+2	NL1K1	NL1K1=number of entries in the level 1 χ_1-table;
⋮	⋮	
LOCKL1+2*NMXL1K+1	NL1KN	NL1KN=number of entries in the level 1 χ_{NMXL1K}-table;
(End Level 1 T-Table)		
⋮		
LOCKLN	LEVEL NLEV T-TABLE	LEVEL NLEV T-TABLE is exactly analogous to the level 1 T-TABLE;
LOCCON	NMXENN	NMXENN=maximum number of E' entries in an ENN table;
LOCCON+1	LCENN1	LCENN1 =pointer for the E'_1 table;
⋮	⋮	
LOCCON+NMXENN	LCENNM	LCENNM=pointer for E'_{NMXENN} table;
LOCCON+NMXENN+1	NEP1	NEP1=number of entries in the E'_1 table;
⋮	⋮	
LOCCON+2*NMXENN	NEPN	NEPN=number of entries in the E'_{NMXENN} table;
LOCCON+2*NMXENN+1	LCKEP1	LCKEP1=pointer for the T-table corresponding to E'_1;
⋮	⋮	
LOCCON+3*NMXENN	LCKEPN	LCKEPN=pointer for the T-table corresponding to E'_{NMXENN};
LCKEP1	E'_1 T-TABLE	The E' T-Tables are analogous in structure to the level T-tables;
⋮	⋮	
LCKEPN	E'_{NMXENN} T-TABLE	

(Start Basic Energy Table)

LOCATION	CONTENTS	COMMENTS
LCETAB+1	E_1	E_1=first (highest) energy in the basic energy table;
⋮	⋮	
LCETAB+NEN	E_{NEN}	E_{NEN}=NENth (lowest) energy in the basic energy table;
(End Basic EN TABLE) (Start Elastic CHI EN Table)		
LCENEK+1	EEK_1	EEK_1=first (highest) energy in the elastic chi energy table;
⋮	⋮	
LCENEK+NENEK	EEK_{NENEK}	EEK_{NENEK}=last (lowest) energy in the elastic chi energy table;
(End Elastic CHI EN Table) (Start Level 1 CHI EN Table)		
LCEL1K+1	$EL1K_1$	$EL1K_1$=first (highest) energy in the level 1 chi energy table;
⋮	⋮	
LCEL1K+NENL1K	$EL1K_{NENL1K}$	$EL1K_{NENL1K}$=last (lowest) energy in the level 1 chi energy table;
⋮	⋮	
LCELNK+1	LEVEL NLEV CHI EN. TABLE	LEVEL NLEV energy table is exactly analogous to the level 1 energy table;
LCEP1K+1	E'_1 CHI EN. TABLE	The E' chi energy tables are analogous to the level chi energy tables;
⋮	⋮	
LCEPNK+1	E'_{NMXENN} CHI EN. TABLE	
LOCT+1	$SIGT_1$	$SIGT_1$=first total cross section (corresponding to first basic energy);
⋮	⋮	
LOCT+NEN	$SIGT_{NEN}$	$SIGT_{NEN}$=last entry in the total cross cross section table;
LOCS+1	$SIGS_1$	$SIGS_1$=first total scattering cross section entry;
⋮	⋮	

LOCATION	CONTENTS	COMMENTS
LOCS+NEN	$SIGS_{NEN}$	$SIGS_{NEN}$=last entry in the total scattering cross section table;
LOCI+1 . . . LOCI+NI	$SIGIN_1$ . . . $SIGIN_{NI}$	$SIGIN_1$=first entry in the total inelastic cross section table; $SIGIN_{NI}$=last entry in the total inelastic cross section table;
LOCM+1 . . . LOCM+NM	ULT_1 . . . ULT_{NM}	ULT_1=first entry in the multiplicity table; ULT_{NM}=last entry in the multiplicity table;
LOCEK1+1 . . . LOCEK1+NEK1 . . . LOCEKN+1 . . LOCEKN+NEKN	$X1E_1$ . . . $X1E_{NEK1}$ . . . XNE TABLE	$X1E_1$=first entry in the elastic χ_1 table; $X1E_{NEK1}$=last entry in the elastic χ_1 table; XNE TABLE is the elastic χ_{NMXEK} table;
LCL1K1+1 . . . LCL1KN+NL1KN . . . LCLNK1+1 . . . LCLNKN+NLNKN	XL1 TABLES XLNLEV TABLES	XL1 TABLES are the χ-tables for level 1; XLNLEV TABLES are the χ-tables for level NLEV;
LCP1K1+1 . . . LCPNKN+NPNKN	ENN χ-Tables	The ENN χ-tables are stored in an analogous manner;
LOCL1+1 . . . LOCL1+NL1	$SIGL1_1$ . . . $SIGL1_{NL1}$	$SIGL1_1$=first entry in the level 1 cross section table; $SIGL1_{NL1}$=last (threshold) entry in the level 1 cross section table;

LOCATION	CONTENTS	COMMENTS
LOCL2+1 ⋮	$SIGL2_1$ ⋮	$SIGL2_1$=first entry in the sum through level 2 cross section table;
LOCL2+NL2	$SIGL2_{NL2}$	$SIGL2_{NL2}$=last entry in the sum through level 2 cross section table;
LOCLN+NLN	$SIGLN_{NLN}$	$SIGLN_{NLN}$=last entry in the sum through level NLEV cross section table;
LCENN1+1 ⋮	$ENN1_1$ ⋮	$ENN1_1$=first E_1' value entered in the ENN1 table;
LCENN1+NEP1	$ENN1_{NEP1}$	$ENN1_{NEP1}$=last E_1' value entered in the ENN1 table;
LCENN2+1 ⋮	$ENN2_1$ ⋮	$ENN2_1$=first E_2' value entered in the ENN2 table;
LCENN2+NEP2 ⋮	$ENN2_{NEP2}$ ⋮	$ENN2_{NEP2}$=last E_2' value entered in the ENN2 table;
LCENNM+NEPN =NLENTH	$ENNM_{NEPN}$	$ENNM_{NEPN}$=last E'_{NMXENN} value entered in the ENNM table; (end of EDT for this element; the remainder of the present block of 510 words is filled with dummy entries)

EXPLANATORY REMARKS

1. The FORTRAN rules for implicit designation of variable type have been used in naming the variables.

2. All energy dependent data are tabulated on the basic energy mesh, except for angular distribution chi tables, which may be tabulated on their own energy meshes.

3. The number of total cross section entries, as well as the number of total scatter cross section entries, equals the number of basic energy entries (hence only the number of energies is given explicitly).

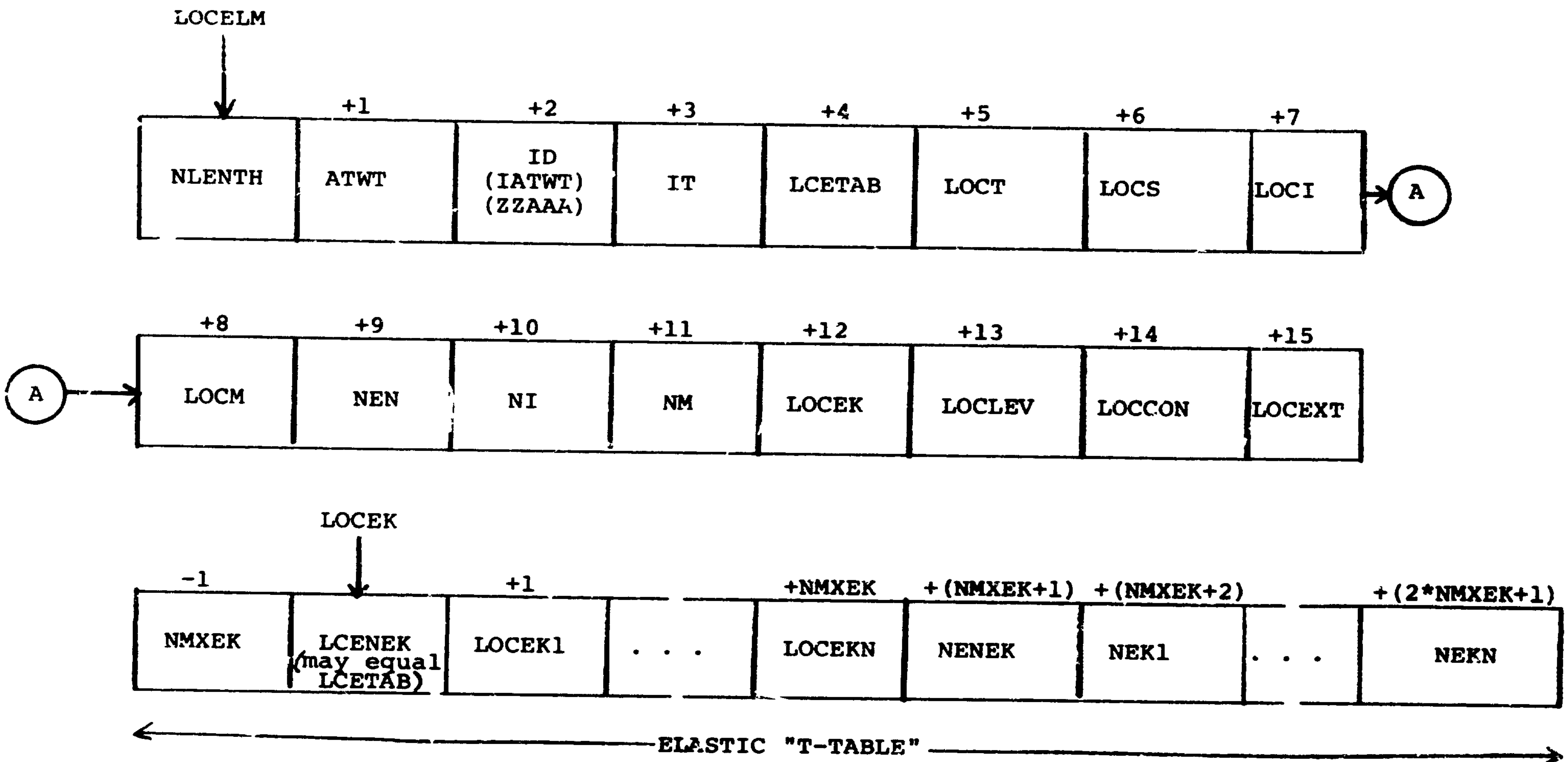
4. All energy dependent data is tabulated in decreasing order of energies.

5. Location pointers having values <1 imply that the corresponding sections do not exist.

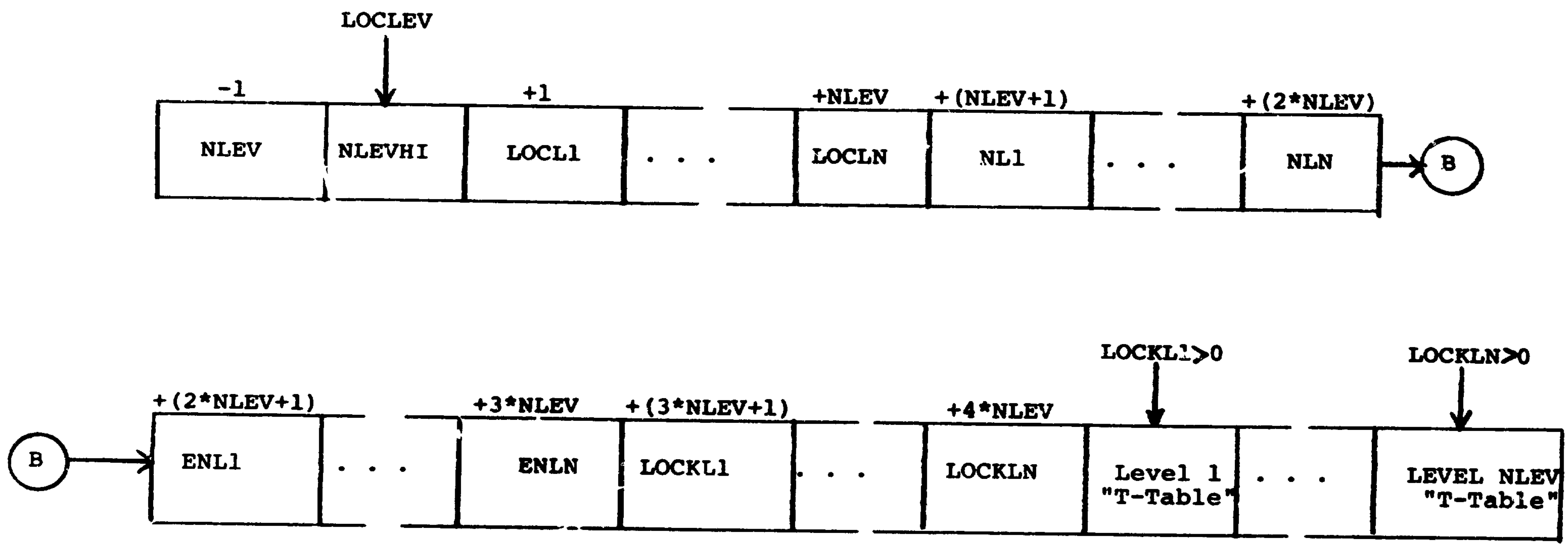
6. Entry numbers <1 imply that the corresponding tables do not exist.

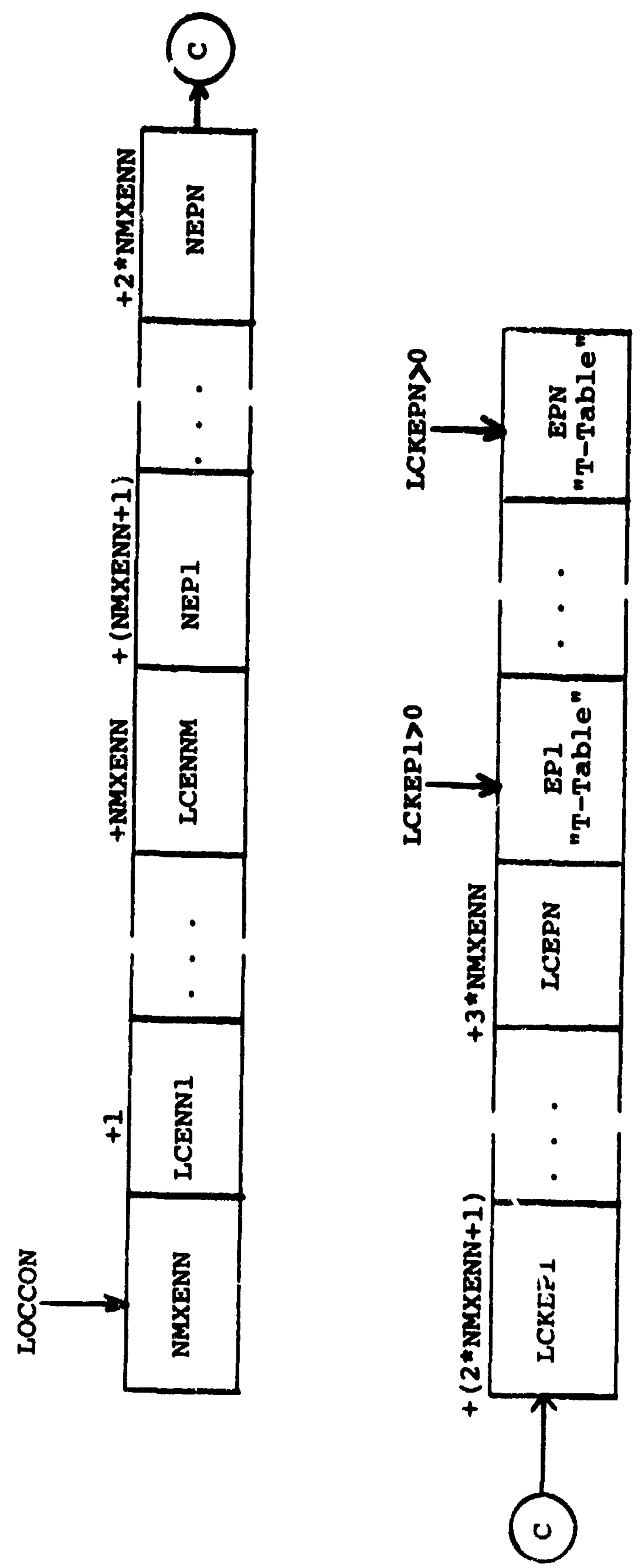
7. LCENEK may be the same as LCETAB (if elastic chi tables have been tabulated on the basic energy mesh).

8. A relative addressing scheme has been simulated in the organization of the neutron EDT through the use of "pointers". A pointer, as here employed, is an address (or word position relative to the start of the data for a given element) with respect to which a table or a specific sequence of entries may be found.



ORGANIZATION CHART FOR NEUTRON ELEMENT DATA TAPE

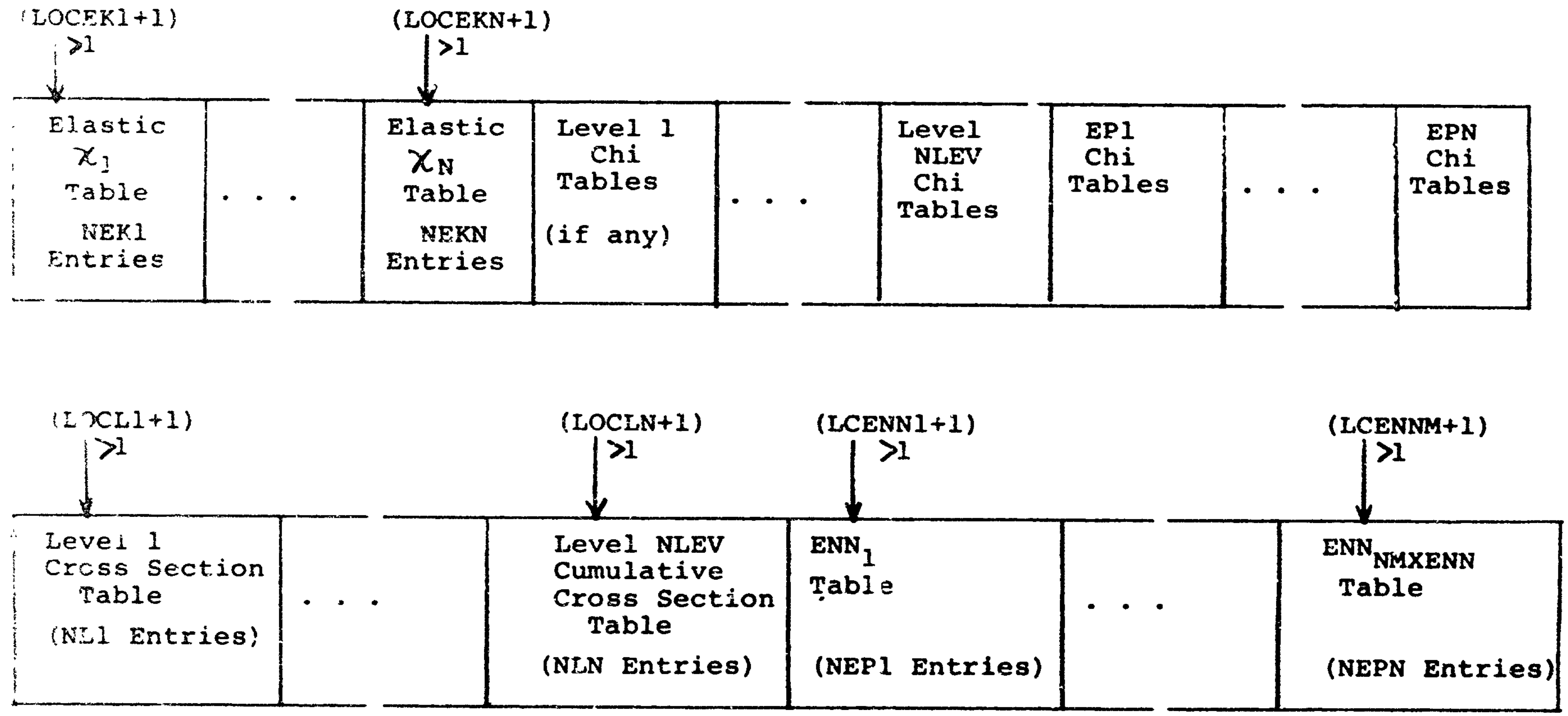

LOCLEV
-1
+1
+NLEV
+(NLEV+1)
+(2*NLEV)
NLEV
NLEVHI
LOCL1
. . .
LOCLN
NL1
. . .
NLN
B
LOCKL1>0
LOCKLN>0
+(2*NLEV+1)
+3*NLEV
+(3*NLEV+1)
+4*NLEV
B
ENL1
. . .
ENLN
LOCKL1
. . .
LOCKLN
Level 1
"T-Table"
. . .
LEVEL NLEV
"T-Table"



LOCCON
NMXENN
+1
LCENN1
. . .
+NMXENN
LCENNM
+(NMXENN+1)
NEP1
. . .
+2*NMXENN
NEPN
C
+(2*NMXENN+1)
LCKEP1
. . .
+3*NMXENN
LCEPN
LCKEP1>0
EP1 "T-Table"
. . .
LCKEPN>0
EPN "T-Table"

(LCETAB+1)	(LCENEK+1) ≥ 1		
Basic Energy Table NEN Entries	Elastic Chi Energy Table NENEK Entries	Level Chi Energy Tables (if any)	Continuum Chi Energy Tables (if any)
	Exists only if LCENEK$\neq$LCETAB		

(LOCT+1)	(LOCS+1)	(LOCI+1) ≥ 1	(LOCM+1) ≥ 1
Total Cross Section Table NEN Entries	Scattering Cross Section Table NEN Entries	Inelastic Cross Section Table NI Entries	Multiplicity Table NM Entries



(LOCEK1+1)
>1
Elastic χ1 Table
NEK1 Entries
. . .
(LOCEKN+1)
>1
Elastic χN Table
NEKN Entries
Level 1 Chi Tables
(if any)
. . .
Level NLEV Chi Tables
EP1 Chi Tables
. . .
EPN Chi Tables
(LOCL1+1)
>1
Level 1 Cross Section Table
(NL1 Entries)
. . .
(LOCLN+1)
>1
Level NLEV Cumulative Cross Section Table
(NLN Entries)
(LCENN1+1)
>1
ENN1 Table
(NEP1 Entries)
. . .
(LCENNM+1)
>1
ENNNMXENN Table
(NEPN Entries)

APPENDIX B

Organization of the Gamma Element Data Tape (GEDT)

The gamma ray element data tape is created by program SAM-X. It may be made one or several elements at a time with the same SAM-X run. Each elemental set of data on the tape is written as a series of logical binary records, each 510 words long. The number of such records for an element is given, in fixed point arithmetic, by:

$$\frac{(\mathrm{NLENTH}-1)}{510} + 1$$

Where NLENTH is the number of words of data for the element. Usually, NLENTH<510, and thus each element requires only one binary record.

In principle, the organization of the gamma ray data tape is identical to the neutron data tape. However, most of the optional extra pointers, indices and tables of the neutron tape (see Appendix A) are replaced by default zero values for the gamma ray tape. Thus the gamma ray data files are, in reality, of a much more simple nature than are the neutron files.

The following is a description and a map of the organization and contents of the gamma element data tape for one element.

LOCATION	CONTENTS	COMMENTS
1st word	NLENTH	NLENTH=number of words of data for this element.
2nd word	ATWT	ATWT=atomic weight
3rd word	ID	ID=the ZZAAA designation for the material (not the ENDF MAT #).

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LOCATION	CONTENTS	COMMENTS
4th word	IT	IT is currently ignored
5th word	LCETAB	LCETAB = pointer to the energy table
6th word	LOCT	LOCT = pointer to the total cross section table*
7th word	LOCS	LOCS = pointer to the scattering cross section table **
8th word	--	always zero
9th word	--	always zero
10th word	NEN	NEN = number of words in the energy table
11th - 16th words	--	always zero
LCETAB+1 ⋮	E_1 ⋮	E_1 = first (highest) energy
LCETAB+NEN	E_{NEN}	E_{NEN} = NEN th (lowest) energy
LOCT+1 ⋮	$SIGT_1$ ⋮	$SIGT_1$ = first total cross section (corresponding to E_1)
LOCT+NEN	$SIGT_{NEN}$	$SIGT_{NEN}$ = NEN th total cross section (corresponding to E_{NEN})
LOCS+1 ⋮	$SIGS_1$ ⋮	$SIGS_1$ = first scattering cross section (corresponding to E_1)
LOCS+NEN	$SIGS_{NEN}$	$SIGS_{NEN}$ = NEN th scattering cross section (corresponding to E_{NEN}); (end of this element; the remainder of the present block of 510 words is filled with dummy entries).

* Coherent scattering for photons is not treated by SAM-F or SAM-A. Hence, the total cross section has been reduced by the coherent scattering cross section. Work is currently underway to provide full x-ray treatment. This will be available when Revision D is issued.

** Incoherent scattering only.

APPENDIX C

Structure of the Organized Data Tape (ODT)

Subroutine BAND and its subsidiary routines read in cross section data from the element data tape (EDT), and composition descriptions (i.e., elemental concentrations) from the input data cards. These data are then combined into the organized data tape (ODT-Tape 10) which is used in the Monte Carlo game as the supplier of cross sections and to determine post-collision energies and angles of scattering. If desired, the ODT may also be saved for subsequent Monte Carlo problems involving the same compositions.

In general, the code splits the data into NBAND number of cross section bands. NBAND, as well as the energy band limits, are automatically determined by the code, unless the user desires to enter these data as input.

Each of the NBAND bands, placed on the tape in order of decreasing energy, are similar in format and contain the cross section data appropriate to the range.

The structure for each of the bands is as follows:

Item 1

1.1 Band number

1.2 1 plus band number

1.3 Upper energy limit of band

1.4 Lower energy limit of band

1.5 1 plus maximum size of any band (i.e., the required core allocation for cross sections).

1.6 Number of bands

1.7 Length of current band

The rest of the items are packed into the MASTER array.

Item 2 (repeated NCOMP times)

2.1 Location of the concentration of the first element in composition 1

2.2 Location of the concentration of the first element in composition 2

⋮

2.NCOMP Location of the concentration of the first element in composition NCOMP

Item 3 (Location NCOMP+1)

3.1 2 plus the location of the concentration of the last element of the last composition. Also points to start of first stored elemental data

Item 4 (starts in Location NCOMP+2)

Item 4 consists of two entries, repeated for each element in composition 1, next repeated for each element in composition 2, etc., until they are repeated for each element in composition NCOMP.

4.1 Concentration of this element in this composition.

4.2 Start of elemental data for this element.

Note, if an element is repeated in two or more compositions, Item 4.2 will point to the same location for each repetition.

Item 5 Appears for each element treated in the problem. For repeated elements it appears only once.

Item 5 is essentially the cross section data from the element data tape truncated for the energy range of the present band.

As an option, the user may obtain a complete printout of the ODT, band by band. Due to the relatively small amount of data involved, gamma ray ODT's usually consist of only one band. If gamma ray production data is desired, in addition to gamma ray cross sections, only one band is currently allowed. This restriction will be removed in the near future.

APPENDIX D

Organization of the Gamma Ray Production Data Tape (GPDT)

LOCATION	CONTENTS	REMARKS
1st word	LENGTH	total number of words for this element;
2nd word	ATWT	atomic weight;
3rd word	ID	element identifier; ZZAAA
4th word	LCENTB	pointer for basic energy table;
5th word	NEN	number of entries in basic energy table;
6th word	LOCEG	pointer for photon information;
7th word	LOCEXT	pointer for additional information (if needed);
LOCEG	NEG	number of photon energies;
LOCEG+1	LCG1	pointer for 1st photon yields;
.	.	
LOCEG+NEG	LCGNEG	pointer for yields for last photon;
LOCEG+NEG+1	MG1	starting energy mesh point for first photon yields;
LOCEG+NEG+2	NG1	last energy mesh point for first photon yields;
.	.	
LOCEG+3*NEG-1	MGNEG	starting energy mesh point for last photon yields;
LOCEG+3*NEG	NGNEG	last energy mesh point for last photon yields;
LOCEG+3*NEG+1	EG1	first photon energy;
.	.	
LOCEG+4*NEG	EGNEG	last photon energy;
LOCEG+4*NEG+1	KG1	pointer for ang. dist. inform. for first photon;
.	.	

LOCATION	CONTENTS	REMARKS
LOCEG+4*NEG+L	KGL	pointer for ang. dist. inform. for L-th photon;
⋮	⋮	
LOCEG+5*NEG	KGNEG	pointer for ang. dist. inform. for last photon;
(Start of T-TABLE* for L-th Photon)		
KGL (> 0)	MXK	maximum number of chis for L-th photon
KGL+1	LCEKTB	pointer for chi energy table;
KGL+2	LCK1	pointer for chi 1 table;
⋮	⋮	
KGL+MXK+1	LCKMXK	pointer for last chi table;
KGL+MXK+2	NE	number of chi energies;
KGL+MXK+3	NK1	number of chi 1 entries;
⋮	⋮	
KGL+2*MXK+2	NKMXK	number of entries in last chi table;
(End of T-TABLE for L-th photon)		
LCENTB+1	NEN neutron energies	
⋮	⋮	
LCEKTB+1	NE chi energies	only if KGL>0;
⋮	⋮	
LCK1+1	NK1 chi 1 entries	only if KGL>0;
⋮	⋮	
LCG1+1	(NG1-MG1+1) multiplicities for EG1	
⋮	⋮	
LCGNEG+1	(NGNEG-MGNEG+1) multiplicities for EGNEG	

---

* A T-TABLE summarizes the fixed point information (i.e., pointers and numbers of entries) for each photon, provided anisotropic information is given (as would be flagged by KGL>0, L=1,...,NEG).

Dummy GPDT

It sometimes occurs that the user wishes to include a nuclide in the secondary gamma ray calculation which was not present in the primary neutron problem, e.g., argon for air transport problems. Also, he may wish, for some reason, to suppress gamma production from a specific nuclide (or nuclides) in order to assess certain effects.

These goals are best accomplished by generating and using dummy GPDT's for the nuclides in question. Denoting ID as the proper ZZAAA (see "3rd word", above) the following *ad hoc* program may be used:

```
      PROGRAM DUMMY (TAPE15)
      DIMENSION I(510)
      DO 10 J=1,510
   10 I(J)=0
      I(1)=8
      I(3)=ID     ← enter proper numeric value here
      I(6)=8
      WRITE(15) I
      END
```

The output will be on TAPE15 - the same as for a true SAM-X run (Section 2.7).

APPENDIX E

Energy Hierarchy - SAM-F

The Monte Carlo transport is run between EHIGH and ECUT.

Then,

$EOUT_1 > EHIGH$	$EOUT_{LAST} < ECUT$
$ES_1 > EHIGH$	$ES_{LAST} < ECUT$
$EWTAB_1 > EHIGH$	$EWTAB_{LAST} < ECUT$

where EOUT = output score energies

ES = source energies

EWTAB = energies for energy importance sampling

Note: There is no hierarchy required among EOUT, ES and EWTAB.

ALSO

$EDATA_1 > EX_1 > EHIGH$	$EDATA_{LAST} < EX_{LAST} < ECUT$

where EDATA are the energy limits for the element on the element data tape (TAPE 11). If several "i-th" elements are involved, $EDATA_1$ is the lowest of all the $EDATA_{1,i}$ values and $EDATA_{LAST}$ is the highest of all $EDATA_{LAST,i}$.

EX are the cross section limits specified when creating the organized data tape (TAPE 10), i.e., when running BAND.

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APPENDIX F

Discussion of Importance Sampling

It is fairly well known [1] that Monte Carlo calculations can be carried out so that a single linear functional (e.g., dose, Fe activation) of the radiation field may be calculated with zero variance. To do this one requires pre-knowledge of an "importance function" which gives for any particle its expected contribution to that single functional. This importance function is used to bias histories of particles so as to direct them toward those positions, energies, and directions at which the chance of contributing to an answer is large. In addition, to get strictly zero variance it is necessary to compute an answer (to "score") only when an importance modified history is terminated.

To be more explicit, let $\underset{\sim}{x}$, E, $\underset{\sim}{\Omega}$ denote the position, energy, and direction of a particle and let $J(\underset{\sim}{x},E,\underset{\sim}{\Omega})$ be the expected total answer eventually given by that particle. Then if $K(\underset{\sim}{x}',E',\underset{\sim}{\Omega}'\rightarrow\underset{\sim}{x},E,\underset{\sim}{\Omega})$ is the density of particles coming out of collisions at $\underset{\sim}{x},E,\underset{\sim}{\Omega}$ given that one came into a collision at $\underset{\sim}{x}',E',\underset{\sim}{\Omega}'$ define the altered kernel

$$\tilde{K}(\underset{\sim}{x}',E',\underset{\sim}{\Omega}'\rightarrow\underset{\sim}{x},E,\underset{\sim}{\Omega}) = J(\underset{\sim}{x},E,\underset{\sim}{\Omega}) \times K(\underset{\sim}{x}',E',\underset{\sim}{\Omega}'\rightarrow\underset{\sim}{x},E,\underset{\sim}{\Omega})/$$

$$\left\{\iint J(\underset{\sim}{x}'',E'',\underset{\sim}{\Omega}'') \times K(\underset{\sim}{x}',E',\underset{\sim}{\Omega}'\rightarrow\underset{\sim}{x}'',E'',\underset{\sim}{\Omega}'')\,d\underset{\sim}{x}''dE''d\underset{\sim}{\Omega}''\right\} .$$

This kernel is to be used in generating histories if zero variance is to be obtained. Another requirement is that the source density $\tilde{S}(\underset{\sim}{x},E,\underset{\sim}{\Omega})$ be replaced by

$$S(\underset{\sim}{x},E,\underset{\sim}{\Omega}) = J(\underset{\sim}{x},E,\underset{\sim}{\Omega})S(\underset{\sim}{x},E,\underset{\sim}{\Omega})/\int J(\underset{\sim}{x}',E',\underset{\sim}{\Omega}')S(\underset{\sim}{x}',E',\underset{\sim}{\Omega}')\,d\underset{\sim}{x}'dE'd\underset{\sim}{\Omega}'$$

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in selecting starting coordinates for histories.

In practice, the conditions for obtaining zero variance are never achieved for any practical problem. It is useful to note the reasons.

1. The exact importance function is never known. If it were, the exact answer to the problem would be known.

2. Scoring is carried out during the history, and not only at its end as required for zero variance calculation.

3. It is difficult to represent the space, angular, energy, and time dependence of even approximate importance functions in sufficient detail.

4. Renormalization of the altered kernel $\tilde{K}$ and sampling from it is a time consuming process. General purpose codes implement alternative methods such as splitting at boundaries. This always increases the variance.

The first point is a difficulty in principle. In practical problems, it has been found that approximate forms for J can reduce the variance in difficult problems to the point where modern computing machines can achieve satisfactory results. Several methods have been used to establish the function J. Kalos [2] used a multi-collision approach (essentially consideration of the Neumann series of the adjoint problem) and was able to calculate very deep penetration. At the other extreme, Cain [3] has used S_n codes to find numerical values of J. Unfortunately for two- or three-dimensional problems this requires computations as extensive, or more so than the Monte Carlo calculations themselves. Finally, it is possible to use existing results for similar problems (e.g., moments method

results for gamma rays) as one does in obtaining rough engineering approximations to shielding results themselves. This appears to be the most practical and will be illustrated later.

It has been shown that the essential part of the variance reduction is the use of a properly biased altered kernel and that the particular scoring scheme is less important. [4]

In many codes the importance sampling depends only upon space or occasionally on energy. This, coupled with the fact that extra variance arises in sampling the altered kernel, may well have the effect that the optimum parameters cannot be easily deduced from even a reasonable guess for J. In particular, the failure to alter the source distribution consistent with the history biasing requires special treatment.

The properties of SAM-F are such that the optimum use of the code should result by using a set of weights inversely proportional to $J(\underset{\sim}{x},E,\underset{\sim}{\Omega})$. These weights can depend upon position, energy, and direction. The source spectrum is altered automatically according to the weights. Finally, the biased histories, particularly the flight of a particle, are carried out so as to provide little additional variance.

Thus establishing efficient sampling reduces to calculating a reasonable approximation to J. Before giving an example, certain general remarks can be made.

First, because the importance function is specified through weights that are constant in spatial regions, the requirements of biasing reflect upon the geometry used to describe the problem. Thus an effort should be made to provide enough regions so that in significant regions of space, and for the part of the spectrum responsible for penetration to the detector, the variation in average importance from one region to the next is no more than (very roughly) a factor of four. This requirement can be relaxed for regions far from source and detector or for radiation too weakly penetrating or too weak to enter into the further penetration.

The use of appropriate symmetries simplifies the importance sampling. Although, in principle, a result can be obtained as easily in a small region as in a shell in a spherically symmetric problem, in practice extra care must be given to focus the radiation appropriately toward a small detector. This is done in the SAM-F bounded estimator procedure. For a shell surrounding a spherical source, only the exponential attenuation with position is needed.

When a reasonable set of weights has been given for a set of detectors in a given geometry, it can be used for a variety of sources. Thus a good set of importance weights for gamma rays in a given situation can be used for monoenergetic gammas, for a prompt fission gamma source, or for spatially and energy-distributed gammas arising from neutron interactions. Naturally, if space or energy regions previously thought unimportant are no longer so, extensions must be made.

In some problems it is necessary (or thought necessary) to obtain several different answers in a single computer run. If these answers depend essentially upon the same or very similar histories, (as for example, the biological dose at two detectors separated by less than a relaxation length for the dominant radiation), then a biasing scheme for one (or for a detector at a mean position) does reasonably well for the other. When rather different histories are required (as for widely separated detectors or for neutron dose contrasted with sources of secondary gamma radiation) then it may well be true that separate runs with separate importance weights will be computationally most efficient. In intermediate cases where it is suspected that the computational gain from running a single problem is important, the following prescriptions are useful.

1. Take weights proportional to flux over the important range of position and energy. This has the effect of giving generally good statistics for flux over that range (though likely at the expense of computing time). The numerical values of flux may be taken from related problems or from a preliminary run.

2. Take the spatial dependence of weight proportional to the expected dose over regions of adjacent detectors. Outside regions of detectors compute relative importance for nearest detector.

3. Take a linear combination of the importance function for single detectors, the coefficient being inversely proportional to the estimated result at that detector. The weight is, of course, inversely proportional to the composite importance.

Note that in SAM-F the magnitude of the weight is irrelevant.

Finally we give the following warning. It is often tempting to try a rather sharp biasing, particularly in direction. It should always be kept in mind that the importance function is the expected answer after all future collisions, not just a single one. Thus a particle pointed within some neighborhood of a detector (e.g., within a cone that passes as close as roughly a mean free path for scattered radiation) is likely to be nearly as important as a ray that passes directly through. Neglect of this leads to biasing in which the most probable result, except in very long sampling, omits this scattered radiation. In somewhat the same way, radiation directed away from a detector may, in consequence of multiple scattering, be nearly as important as radiation directed toward a detector. When diffusion dominates, there is little direction effect.

The last section will describe the procedure used to set up weights for gamma-ray transport in the atmosphere above a ground interface.

It was required to calculate free air gamma-ray doses in two sets of detectors. The first set consisted of detectors centered at 250, 500, 750 meters and the second at 1000, 1250, 1500 meters. Each set was considered a separate problem. Each "detector"

was in fact a ring of air, 7 meters high, and whose inner and outer radii differed by 20 meters. The rings abutted the ground.

The air was subdivided into large concentric rings, 600 meters high, centered on the source. The increment in radius was taken as 125 meters; this is adequately small compared with the average relaxation length of about 600 meters. Each detector ring was contained in one of the larger rings.

The energy grouping was taken as follows. Energies above 4 Mev were lumped together. Other divisions were taken at 2, 1, 0.5, and 0.2 Mev. Except below the last, the variation in cross-section in a group is less than about 30% so that the importance is reasonably taken to be constant in each group. The properties of gammas were evaluated at the lower end except for the lowest, for which 0.1 Mev was used.

The procedure for establishing weights was the following. Assume we are dealing with the second group of detectors. The effectiveness of a gamma was taken (for calculating importance only) to be proportional to energy. At 1000 meters therefore, the weight was set equal to the reciprocal of the group energy in Mev. From 1000 to 1500 meters the weight was assumed to decrease exponentially (i.e., the importance increased exponentially) with a relaxation length of 550 meters, taken from an earlier calculation as characteristic of dose. The same ratios in weights were used in each energy range. The importance at 500 meters and at 1000 meters was evaluated as $\left[E \cdot B(E) r^{-2} e^{-\mu(E) r}\right]^{-1}$ using r=500 and 1000 meters,

respectively. These are, of course, the distances to the first detector. Buildup factors B(E) were taken for point isotropic sources from Goldstein[5] except at the lowest energies where very rough extrapolations were made. At points 500 meters and 1000 meters beyond the last detector, the weights were made to rise in the same ratios. These points were plotted on semilog paper and curves drawn joining them. This is shown in Figure F.1. Rough average weights are taken directly from the graph.

It is easy to see from this prescription that, for detectors in the range 250 to 750 meters, one may use the same curve by shifting the entire curve left by 750 meters. This is rather generally applicable.

No angular weights were used, primarily because the regions are so large that the assumption of constant preferred direction is not applicable. For this reason (among others) it would have been preferable to subdivide the vertical section by several parallel planes. Since satisfactory answers were obtained in short computing times we did not go in this direction for gammas, although significant improvements were found in using more vertical divisions in neutron problems.

The weights in ground were always taken to be four times the corresponding weights in the air above. Gammas histories were terminated above 600 meters or beyond 1900 meters from the source.

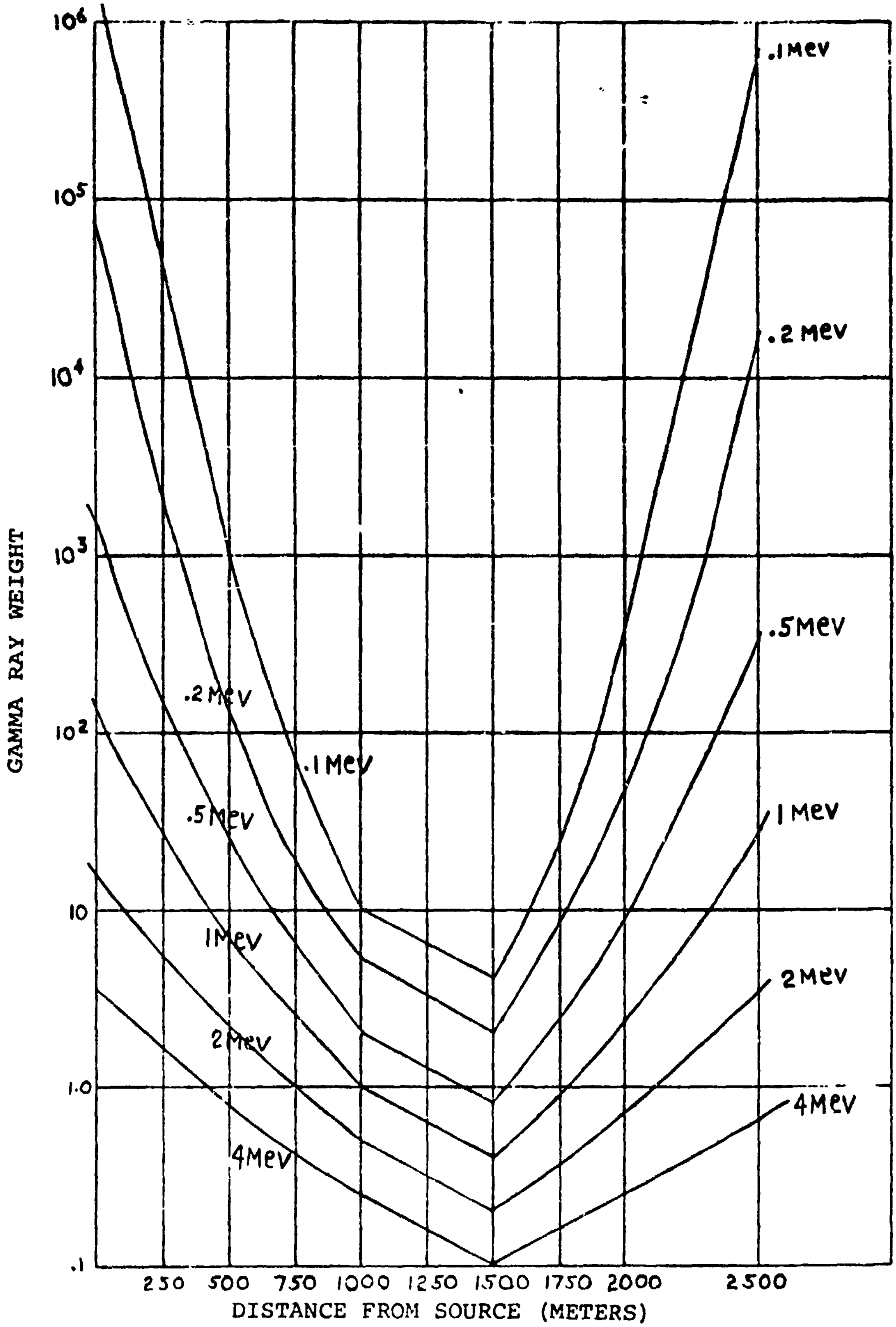

Fig. F. 1 - Gamma Ray Weights vs Distance from Source for Detectors in 1000 to 1500 Meter Range

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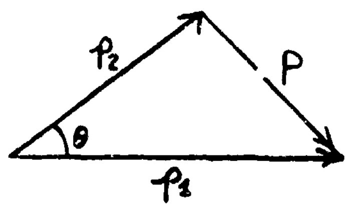
APPENDIX G

Effect of Neglecting Relativistic Changes in SAM-F

Consider an elastic scattering event between a neutron of rest energy $\frac{1}{2}r$ and a nucleus of rest energy $\frac{1}{2}Ar$, where A is the rest mass of the nucleus in units of neutron mass.

Let E_1 and E_2 be the initial and final kinetic energies of the neutron, respectively. Then, if θ is the angle of scattering in the lab, the relativistic mechanics of the event may be represented by a momentum vector diagram:



where p_1, p_2, P are the magnitudes of the "space" components for the incoming and outgoing neutron and recoil nucleus, respectively.

Invoking the conservation of 4-vector momentum yields:

$$c^2p_1^2 = E_1^2+rE_1 \tag{G.1a}$$

$$c^2p_2^2 = E_2^2+rE_2 \tag{G.1b}$$

$$c^2P^2 = (E_1-E_2)^2 + Ar(E_1-E_2) \tag{G.1c}$$

(relations easily derived from, for instance, Leighton, Principles of Modern Physics, pp. 34-37).

Letting $\omega = \cos\theta$, the law of cosines yields:

$$P^2 = P_1^2+P_2^2-2P_1P_2\omega \qquad \text{(G.2)}$$

Rearranging equation (G.2) and squaring both sides

$$4\omega^2P_1^2P_2^2 = P_1^4+P_2^4+2P_1^2P_2^2+P^4-2P^2(P_1^2+P_2^2) \qquad \text{(G.3)}$$

Substituting equations (G.1a,b,c) into equation (G.3) yields, after canceling common terms and rearranging

$$a_1E_2^2+a_2E_2+a_3 = 0 \qquad \text{(g.4)}$$

where the coefficients of the quadratic equation are given by

$$a_1 = 4(1-\omega^2)E_1^2+(A+1)^2r^2+4(1-\omega^2+A)rE_1 \qquad \text{(G.5a)}$$

$$a_2 = 4(1-\omega^2-A)rE_1^2+2(1-A^2-2\omega^2)r^2E_1 \qquad \text{(G.5b)}$$

$$a_3 = (A-1)^2r^2E_1^2 \qquad \text{(G.5c)}$$

Letting $T = E_2/E_1$:

$$T = \frac{4(\omega^2+A-1)rE_1+2(2\omega^2+A^2-1)r^2+4r\omega(E_1+r)\sqrt{\omega^2-1+A^2}}{2(A+1)^2r^2+8(1-\omega^2)E_1^2+8(1-\omega^2+A)rE_1} \qquad \text{(G.6)}$$

where we have retained the root which yields T=1 for $\omega=1$ (recall that the additional root was introduced by squaring equation (G.2)).

Letting $\rho = E_1/r$, equation (G.6) becomes

$$T(\rho) = \frac{b_1+b_2\rho}{b_3+b_4\rho+b_5\rho^2} \tag{G.7}$$

where the coefficients are given by

$$b_1 = 2\omega^2+A^2-1+2\omega\sqrt{\omega^2-1+A^2} \tag{G.7a}$$

$$b_2 = 2(\omega^2-1+A)+2\omega\sqrt{\omega^2-1+A^2} \tag{G.7b}$$

$$b_3 = (A+1)^2 \tag{G.7c}$$

$$b_4 = 4(1-\omega^2+A) \tag{G.7d}$$

$$b_5 = 4(1-\omega^2) \tag{G.7e}$$

Expanding equation (G.7) in powers of ρ and keeping terms to order ρ yields:

$$T(\rho) \simeq T_o + \left\{ \frac{2(\omega^2-1+A)+2\omega\sqrt{\omega^2-1+A^2}}{(A+1)^2} - T_o \left[\frac{4(1-\omega^2+A)}{(A+1)^2} \right] \right\} \rho \tag{G.8}$$

where the non-relativistic energy ratio T_o is given by

$$T_o = T(o) = \frac{b_1}{b_3} = \frac{2\omega^2+A^2-1+2\omega\sqrt{\omega^2-1+A^2}}{(A+1)^2} \tag{G.9}$$

For $A >> 1$, equation (G.8) becomes

$$T(\rho) \simeq T_o + \left[\frac{2(1+\omega)}{A} - \frac{4}{A} T_c\right]\rho \qquad \text{(G.10)}$$

For $A = 1$ and $\omega \geq 0$, equation (G.8) becomes

$$T(\rho) \simeq T_o + \left[\omega^2 - (2-\omega^2) T_o\right]\rho \qquad \text{(G.11)}$$

Example

Given: $E_1 = 20$ Mev, $\omega = -1$;

Substituting $\omega = -1$ into equation (G.8) yields

$$T(\rho) \simeq T_o \left[1 - \frac{4A}{(A+1)^2}\rho\right]$$

$\rho = E_1/r$ where r = 2x rest energy of a neutron = 2x931 (Mev)

$$\therefore \quad \rho = \frac{20 \text{ Mev}}{2 \times 931 \text{ Mev}} = \frac{10}{931}$$

$$T/T_o = 1 - \left[4.30 \times 10^{-2} \times \frac{A}{(A+1)^2}\right]$$

Hence, for A=14, the effect of neglecting the relativistic change is a discrepancy of 0.27%.

APPENDIX H

Organization of the MASTER* Array

The following section describes the organization and contents of the MASTER storage array. The capitalized name in the upper left-hand corner of each box refers to a location relative to start. These locations are used to find sections of data with a minimum of calculation.

ITEM	LOCATION (in capitals) & CONTENTS	COMMENTS
(1)	1 Largest cross section band	See Section 3.2.3.
(2)	LEGEOM 1 blank location	
(3)	LSCORE Region flux scores for each statistical aggregate	The scores are accumulated and stored by CARLO. The scores are stored as a function of energy and scoring region.
(4)	LREGT Region-dependent parameters	This section of the array contains region-dependent parameters stored six computer words per region. Th data are read in and stored by INPUTD.
(5)	LNCOL Number of collisions per region	
(6)	LENDEP The energy deposition per region	
(7)	LNESC The weighted number of escapes and Russian roulette kills per region	

* MASTER and ASTER are equivalenced.

(8)	LCUT The weighted number of escapes, absorptions, and time and energy cuts per region.	
(9)	LNTMDG The number of time cutoffs and degrades per region	
(10)	LNABS The number of absorptions per region	

For items (5) through (10) the starting locations are computed in INPUTD. The counts are accumulated in CARLO and are printed in TALLY.

(11)	LSCFAP Fluxes for all detectors	The scores are computed by FLUP or FLUPV. This section of the array will exist only if detectors are present in the problem.
(12)	LRAW Region weights	The actual region weights to be used for region importance. The weights are read in by INPUTD.
(13)	LREW Region energy weight sets	The energy weight sets for importance sampling. This section exists if energy importance is used in the problem. The data are read in by INPUTD.
(14)	LAIM Aiming angles	The aiming angles for angular importance. Three words per angle denoting direction cosines are stored. The data are read by INPUTD. The array exists only if angular importance is used.
(15)	LAWS Region angular weight sets	The angular weight sets for angular importance. The array exists only if angular importance is used. The data are read by INPUTD.
(16)	KSOUR Source data	The energy, position, and direction data for the source distribution. The data are read in by SOUCAL. If the source is to be generated from an interaction tape this block of data will contain the gamma ray production data instead.

(17)	LLAST Latent storage for supergroups (ends at NDQ)	This section uses up all available room in the MASTER array. Supergroup latents are stored here. Disk files will be used for latent storage if the available room is insufficient.
(18)	NDQ+1 (Forbidden Storage)	

APPENDIX I

Flux and Percentage Error Calculation

There are two ways to measure the average flux, $\bar{\phi}$, in a region, R. One way is to count m(R), the number of interactions in the region, and if N is the number of source particles,

$$\bar{\phi} = \frac{m(R)}{\mu_T(R)N}$$

This method is inefficient when R is a thin region. It is then necessary to use the other method which is called the track length method:

$$\bar{\phi} = \frac{\text{Total distance all particles traveled in R}}{(\text{Volume of R}) \times N}$$

This method is inefficient when R is a thick region. Thus, SAM-F computes average flux per region and per unit energy in each output energy interval using the expected track length method, or exponential estimator.

The source particles are considered in G equal groups of n particles each, such that N = Gn, each group being denoted by g=1, 2,...,G. The statistical aggregate size, n, must be specified in the input. This grouping is made for statisti al purposes. As it will be shown, although the contribution to the average flux of all expected track lengths is cumulative, the contribution to the variance depends on the grouping.

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Let $S_g(R,E^j)$ be the sum of all expected track lengths of particles from the g^{th} group in region R with energy E in the j^{th} output energy interval.

The average expected track length per source particle per unit energy in the j^{th} interval is given by

$$\bar{S}(R,E^j) = \frac{\sum_{g=1}^{G} S_g(R,E^j)}{(E_j - E_{j+1}) x G n}$$

where E_j, E_{j+1} define the j^{th} energy interval.

The average flux per source particle per unit energy in the j^{th} interval in region R is given by

$$\bar{\phi}(R,E^j) = \frac{\bar{S}(R,E^j) W(E^j,R)}{V(R)}$$

where V(R) and $W(E^j,R)$ are the volume and the weight in the j^{th} energy group of region R, respectively. If the energies are given in ev, expected track lengths in cm, and V(R) in cm^3, $\bar{\phi}(E^j,R)$ is obtained in number of particles per ev-cm^2-source particle.

The deviation of the average flux is obtained from

$$\sigma(R,E^j) = \frac{\bar{\phi}(E^j,G)\cdot G}{\sum_{g=1}^{G} S_g(R,E^j)} \left\langle \frac{1}{G-1} \left\{ \frac{\sum_{g=1}^{G} S_g^2(R,E^j)}{G} - \left[\frac{\sum_{g=1}^{G} S_g(R,E^j)}{G} \right]^2 \right\} \right\rangle^{\frac{1}{2}}$$

and the percentage error is simple $\frac{\sigma}{\phi}\cdot 100$.

APPENDIX J

Bounded Biasing in SAM-A

In Section 4.3.8 the expression for the adjoint gamma ray estimator in the point-to-point geometry was derived. The estimator is normally, (i.e., when natural adjoint sampling is used), unbounded in terms of two variables. Specifically, (referring to Figure 4.5), the estimator F is given by

$$F = \frac{G}{R_T\,|\sin\beta|} \tag{J.1}$$

where G is bounded, R_T is the distance between the extended gamma ray track and the source position, and β is the scattering angle required so that the source wavelength and the wavelength along the gamma track are properly matched, that is:

$$\cos\beta \qquad 1+\lambda_s-\lambda \tag{J.2}$$

where λ_s is the source wavelength and λ is the wavelength along the track.

In order to increase the accuracy and rate of convergence of Monte Carlo estimation, it is highly desirable to introduce biased sampling so that F is bounded. Specifically, the selection of the variables defining the adjoint gamma ray history must be biased so that the weight adjustment factor, which would be a multiplicative factor in G, needed to make the Monte Carlo unbiased, compensates for the two singularities.

In the initial stage of the adjoint history, the appropriate biasing can be carried out in a straightforward way. For primary gamma ray problems the source must not be too close to the detector. For secondary problems, the position of the neutron interaction, which becomes position of the gamma ray source, must be biased to handle the inverse square singularity for the uncollided gamma ray estimation. Since R_T can be expressed as:

$$R_T = R|\sin\alpha| \qquad (J.3)$$

where R is the source-detector separation distance and α is the angle between the initial direction out of the detector and the source-detector line, the singularity in $1/R_T$ for the first collided estimate is simply a singularity in $1/|\sin\alpha|$.

The "natural" sampling for the initial direction out of the detector is isotropic (at least for isotropic detectors). Isotropic selection can be carried out by choosing $\cos\alpha$ uniformly between -1 and 1, and by selecting an azimuthal angle, ψ, uniformly distributed between 0 and 2π. To compensate for the singularity, the selection of α should be made uniform in angle between 0 and π, at least near 0 and π, so that a weight adjustment factor proportional to $\sin\alpha$ is needed to make the Monte Carlo history initially isotropic.

To take care of the singularity due to $1/|\sin\beta|$, a procedure similar to the α selection described above should be used. Let $D(\lambda)$ be the detector response as a function of wavelength. The "natural" distribution for photon wavelength out of the detector

is proportional to $D(\lambda)$. Let λ_s be the wavelength out of the source. Then β is defined by equation (J.2). A first collided estimate is possible only if $\lambda_s \leq \lambda \leq \lambda_s + 2$. Therefore the selection of λ would be carried out in two stages. First choose a range between $S_1 = \{\lambda, \lambda_s \leq \lambda \leq \lambda_s + 2\}$ and $S_2 = \{\lambda, \lambda_s + 2 < \lambda\}$. If $\lambda < \lambda_s$, the history gives nothing (there are no photons at energies above the source energy), so that this range can be omitted. If S_2 is chosen, λ is selected using $D(\lambda)$. However, if S_1 is chosen, transform the problem to a β selection. Let

$$h(\beta) = D(1+\lambda_s - \cos\beta) \tag{J.4}$$

Then "natural" sampling is given by the differential

$$\begin{aligned} dP &= h(\beta)d\cos\beta \\ &= h(\beta)\sin\beta d\beta \end{aligned} \tag{J.5}$$

If β is selected using $h(\beta)d\beta$, then the bias adjustment weight, proportional to $\sin\beta$, will exactly compensate for the $1/|\sin\beta|$ factor in the estimator.

When coming out of collision (as opposed to the above described situation out of the detector), the problem is complicated by the fact that the two angles, α and β, cannot be selected independently. This results from the fact that the wavelength λ out of (adjoint) collisions is coupled to the wavelength into collision λ' by:

$$\lambda = \lambda' - 1 + \cos\beta' \tag{J.6}$$

where λ' is the scattering angle, while α must satisfy

$$\cos\alpha = \cos\alpha'\cos\beta' + \sin\alpha'\sin\beta'\cos\psi \qquad (J.7)$$

where α' is the angle between the direction into collision and the collision-source line, and ψ is an azimuth in a cone of angle β' with the before collision direction as axis. By taking a close look at (J.7), we see that for $\sin\alpha'$ or $\sin\beta'$ near 0, $\cos\alpha$ is almost completely coupled to $\cos\beta'$, so that it would not be possible to sample independently α and β, since β is linked to β' by

$$\cos\beta = 2+\lambda_s-\lambda'-\cos\beta' \qquad (J.8)$$

and the singularities could coincide. (Equation (J.8) is obtained by combining (J.2) and (J.6).)

To take care of this problem, it is necessary to introduce the biasing one step earlier in the Monte Carlo, specifically in the selection of the collision position. In the following, the details of the required biasing procedures are described.

The three variables required at a collision are s, the distance from the previous collision, $\Delta' = \cos\beta'$, and ψ. The "natural" distribution is given by:

$$dP = e^{-\int_0^s \mu_t dr}\, k(\lambda,\lambda')\,ds\,d\Delta'\,d\lambda \qquad (J.9)$$

where $k(\lambda,\lambda')$ is the adjoint Klein-Nishina kernel properly normalized, the equation (J.6) gives λ in terms of λ' and Δ'. The singularity in the estimator can then be expressed in terms of s, Δ', and ψ by noting that

$$|\sin\beta| = \sqrt{1-(\Delta'-c)^2} \tag{J.10}$$

where $c = 2+\lambda_s-\lambda$, and

$$R_T = \sqrt{R_o^2\sin^2\psi+x^2(1-\Delta'^2)} \tag{J.11}$$

where R_o is the distance between the source and the before scatter gamma track, and x is given by:

$$x = s-s_o+\Delta' R_o\cos\psi/\sqrt{1-\Delta'^2} \tag{J.12}$$

and s_o is the distance from the previous collision point to the point of minimum distance (to the source) along the before-scatter track.

Singularities in terms of the variables x, Δ', and ψ occur at

(1) $\Delta' = c\pm 1$

(2) $\sin\psi=0$ and $x=0$

(3) $\sin\psi=0$ and $\Delta'=\pm 1$

Observing that $\sin\psi\simeq\psi$ or $\sin\psi\simeq\pi-\psi$ when $\sin\psi$ is near 0, the ψ integration near $\sin\psi=0$ can be estimated from

$$\int_0^{\psi_o} \frac{d\psi}{\sqrt{R^2\psi^2+x^2(1-\Delta'^2)}} = \frac{1}{R_o}\,\ln\left(\frac{R_o\psi_o+\sqrt{R_o^2\psi_o^2+x^2(1-\Delta'^2)}}{|x|\sqrt{1-\Delta'^2}}\right) \tag{J.13}$$

Since our principal concern here is with $x\sqrt{1-\Delta'^2}\approx 0$, (J.13) can be simplified as:

$$\int_0^{\psi_o} \frac{d\psi}{\sqrt{R_o^2\psi^2+x^2(1-\Delta'^2)}} \approx \frac{1}{R_o} \ln\left(\frac{2R_o\psi_o}{|x|\sqrt{1-\Delta'^2}}\right) \qquad (J.14)$$

The integration with respect to x can be carried out near x=0 to give

$$\frac{1}{R_o} \int_0^{x_o} \ln\left(\frac{2R_o\psi_o}{|x|\sqrt{1-\Delta'^2}}\right)dx = \frac{x_o}{R_o}\left[\ln\left(\frac{2R_o\psi_o}{x_o\sqrt{1-\Delta'^2}}\right) -1\right] \qquad (J.15)$$

Finally it can be observed that the Δ' singularities involving $\ln(\sqrt{1-\Delta'^2})$ and $(1-(\Delta'-c)^2)^{-\frac{1}{2}}$ are integrable even if c=0 (the singularities coincide). This can be seen from $\Delta = \Delta'-c$ and $\beta = \cos^{-1}(\Delta)$. As a result:

$$\frac{\ln(\sqrt{1-\Delta'^2})d\Delta'}{\sqrt{1-(\Delta'-c)^2}} = \ln(\sqrt{1-(\cos\beta+c)^2})d\beta \qquad (J.16)$$

which is obviously integrable for $\cos\beta$ near $-c\pm 1$.

Taking into account the range of integration for x and ψ_o, the singularities integrate to A/R_o, where A is insensitive to the geometry. At each step R_T became R_o for the next step, so that the weight adjustment R_T needed to make the estimator bounded also insures that the $1/R_o$ introduced at the next collision biasing is compensated for.

The algorithm has not yet been implemented (except for the initial direction) in the code. The procedure therefore will only be sketched, leaving a full description to the time of actual implementation. The essential steps are:

(1) Select β, using equation (J.16) or an explicitly integrable approximation, taking into account the subrange division (see description out of the detector) and compute Δ'.

(2) Select x, using equation (J.15).

(3) Select ψ, using equation (J.13).

s can then be computed.

Moreover, a reselection technique would be employed, i.e., only if the variables s, Δ', and ψ were such that R_T or $|\sin\beta|$ was too small would the procedure be used. The R_T singularity has to be taken care of at every collision, while the $|\sin\beta|$ singularity is significant only if estimation is possible.

APPENDIX K

Implementation of Importance Sampling and Adjoint Gamma Ray Transport in SAM-A

The basic procedure for carrying out adjoint gamma ray transport in SAM-A is based on a paper by Kalos[1]. The process as used in SAM-A, however, has the additional feature of wavelength dependent importance sampling. The entire procedure is outlined below:

1. Pick λ (the initial detector wavelength) from the normalized probability density function

$$\phi(\lambda)D(\lambda) \Big/ \int_{\lambda_s}^{\lambda_o} \phi(\lambda)D(\lambda)d\lambda$$

$\phi(\lambda)$ = importance function at the detector
$D(\lambda)$ = detector response function
λ_o = wavelength corresponding to the lowest energy
λ_s = wavelength of the source

2. Choose the initial direction, $\underline{\Omega}$, from a distribution biased towards the gamma ray source (Section 4.3.4).

3. Given the wavelength "λ" and the initial direction, "$\underline{\Omega}$", the collision positions along the range are sampled from

$$f(s) = \frac{\phi_{i+1}}{\phi_i} \mu_{+,i} \quad \exp\left[-\int_0^s \mu_T(S')dS'\right]$$

where ϕ_i = the importance functions in region i along the ray.

μ_T = total cross section.

The sampling process is shown below.

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4. **For piecewise constant cross sections compute recursively (in n)**

$$Q_n = \frac{\mu_{+,i}}{\mu_{T,i}}\left[1-\exp(-\mu_{T,1}S_1)\right] + \sum_{i=1}^{n} \frac{\mu_{+,i}}{\mu_{T,i}} \cdot \frac{\phi_1}{\phi_{i-1}} \exp\left(-\sum_{j=1}^{i-1} \mu_{T,j}S_j\right)\left[1-\exp(-\mu_{T,i}S_i)\right]$$

where $(S_1, S_2, \ldots, S_n)$ = successive ray segments in the regions traversed

$$\mu_{+,i} = 3\frac{\tau}{8}\left(\sum_{\text{all } k} Z_k C_{k,i}\right) R_o$$

$$R_o = \int_{\min(\lambda-2,\lambda_S)}^{\lambda} R(\lambda',\lambda)\,\phi(\lambda')\,d\lambda'$$

$$R(\lambda',\lambda) = \left(\frac{\lambda'}{\lambda}\right)^2\left[\frac{\lambda}{\lambda'} + \frac{\lambda'}{\lambda} - 1 + (1-\lambda+\lambda')^2\right]$$

τ = Thompson's unit

Z_k = atomic number of kth nuclide

$C_{k,i}$ = concentration of kth nuclide (atoms/$cm^3 \times 10^{24}$) in the ith region traversed

When

$Q_n \geq \xi$ (a random number)

a collision will be made at a distance "S" within the nth segment given by

$$\xi = Q_{n-1} + \frac{\phi_{n+1}}{\phi_n} \cdot \frac{\mu_{+,n}}{\mu_{T,n}} \exp\left(-\sum_{1}^{n-1} \mu_{T,i}S_i\right)\left[1-\exp(-\mu_{T,n}S)\right]$$

The random number ξ is incremented by 1 and the wavelength before and after scatter, direction before scatter, position of collision, and weight of the particle are stored in a "latent" table. Note that the wavelength after scatter is computed from the biased Klein-Nishina distribution as shown in Appendix L. The collision depositing procedure is then repeated from step 4 above. When the ray has left the geometry a latent is retrieved, the new direction is computed and the particle is continued from step 3 above. When all latents have been processed a new history is begun from step 1.

REFERENCE FOR APPENDIX K

1. M. H. Kalos, Nuc. Sci. and Eng., 33, 284-290 (1968).

APPENDIX L

Procedure for Selection of Wavelength After Collision in SAM-A

For an adjoint collision taking place at wavelength λ, the probability of scattering to the range $(\lambda_j, \lambda_{j+1})$ is given by:

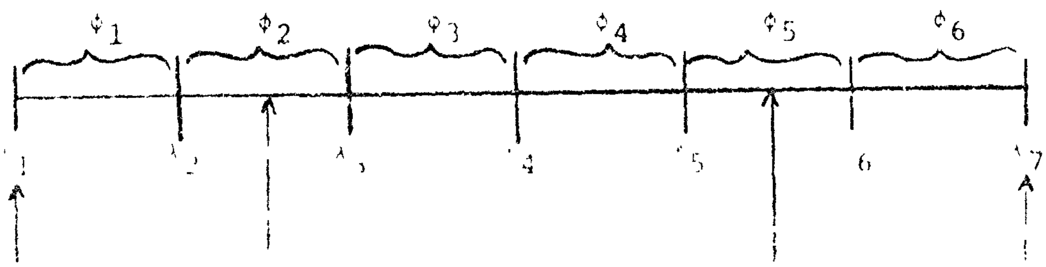
$$p(\lambda_j, \lambda_{j+1}) = \frac{\phi(\lambda_j) \int_{\lambda_j}^{\lambda_{j+1}} R(\lambda', \lambda)\, d\lambda'}{\int_{\lambda_o}^{\lambda} \phi(\lambda') R(\lambda', \lambda)\, d\lambda'}$$

where $R(\lambda', \lambda) = \left(\frac{\lambda'}{\lambda}\right)^2 \left\{ \frac{\lambda}{\lambda'} + \frac{\lambda'}{\lambda} - 1 + (1-\lambda+\lambda')^2 \right\}$

$\phi(\lambda_j)$ = the importance function in the interval $(\lambda_j, \lambda_{j+1})$

and λ_o = $\max(\lambda-2, \lambda_{\text{source energy}})$

The relationship between the various lambdas and the importance function is shown below.



The energy range for the scattering is chosen from "p" and the wavelength after scatter is determined by the following rejection technique:

Let λ_L, λ_U be the wavelength range for the selected interval. For the range (λ_2, λ_3) we would have:

$$\lambda_L = \lambda_o$$

$$\lambda_U = \lambda_3$$

For the range (λ_5, λ_6) we would have

$$\lambda_L = \lambda_5$$

$$\lambda_U = \lambda$$

Given the λ_L, λ_U the rejection procedure is shown below:

$$\text{let} \quad A = \frac{\left\{1+\left(\frac{\lambda_U}{\lambda}\right)^2\right\}^2-4}{\left\{1+\left(\frac{\lambda_L}{\lambda}\right)^2\right\}^2-4}$$

$$\text{and } T = 4-\left\{1+\left(\frac{\lambda_L}{\lambda}\right)^2\right\}^2$$

$$U = \sqrt{\sqrt{4-T\left[A+(1-A)\xi_1\right]}-1} \qquad \text{(L.1)}$$

$$\lambda_{new} = U\cdot\lambda \text{ if } \xi_2\left(U+\frac{1}{U}\right) > 1.-(1-\lambda+\lambda_{new})^2$$

where ξ_1 and ξ_2 are random numbers.

Otherwise, repeat from (L.1).

APPENDIX M

Evaluation of Average Neutron Cross Sections in the Unresolved Resonance Range

A new method is presented for calculating neutron cross sections averaged over the partial width fluctuations in the unresolved resonance range. First, it is shown how the n-dimension integral ($n \le 4$) which appears in the averaging procedure can be reduced to integration in a single dimension. The resulting expression is numerically evaluated by a Gaussian quadrature technique.

M.1 Reduction of the Multidimensional Integral to One Dimension

In the unresolved range the averaged resonance contribution to the neutron cross section is of the form:

$$\sigma_{n,i}^{\ell,J} = \frac{2\pi^2}{k^2} \frac{g_J}{\langle D_{\ell,J} \rangle} \left\langle \frac{\Gamma_i \Gamma_n}{\Gamma} \right\rangle_{\ell,J} \tag{M.1}$$

where

$$\Gamma_i = \Gamma_n, \Gamma_\gamma, \Gamma_f, \Gamma_x, \tag{M.2}$$

$$\Gamma = \Gamma_n + \Gamma_\gamma + \Gamma_f + \Gamma_x, \tag{M.3}$$

and

$$\Gamma_i = \overline{\Gamma}_i r_i / \nu.$$

Here r_i follows the chi-square distribution with ν_i degrees of freedom, i.e.,

$$f_{\nu_i}(r_i)dr_i = \left[2^{\nu_i/2}\Gamma(\nu_i/2)\right]^{-1} r_i^{\nu_i/2-1} e^{-r_i/2} dr_i. \quad \text{(M.4)}$$

Then Equation (M.1) can be written:

$$\sigma_{n,i}^{\ell,J} = \frac{\pi^2}{k^2} \frac{g_J}{\langle D_{\ell,J}\rangle} \frac{\overline{\Gamma}_i\overline{\Gamma}_n}{\overline{\Gamma}\nu_i\nu_n} \int_0^\infty \cdots \int_0^\infty \frac{\nu_i\nu_n}{R_o + \sum_{i=1}^{n} R_i r_i/\nu_i} \pi_i f(r_i)dr_i$$

(M.4)

where,

$R_o = \overline{\Gamma}_o/\overline{\Gamma}$, $R_i = \overline{\Gamma}_i/\overline{\Gamma}$, $1 \le n \le 4$

and $\overline{\Gamma}_o$ is the sum of all non-fluctuating widths.

Note that we have allowed for the possibility of one or more of the widths to remain constant. There may be up to 4 dimensions of integration.

In the following it is shown how the cross section may be reduced to a one-dimensional integral. One must evaluate the multiple integral:

$$J = \int_0^\infty \cdots \int_0^\infty \frac{\prod_{i=1}^{n} dr_i r_i^{(\nu_i/2+m_i-1)} \exp(-r_i/2)}{R_o + \sum_i R_i r_i/\nu_i}, \quad \text{(M.6)}$$

where $m_i = 0$, 1 or 2.

This is accomplished by generalizing J to the form:

$$I(\alpha) = \int_0^\infty \cdots \int_0^\infty \frac{\prod_{i=1}^{n} dr_i r_i^{(\nu_i/2+m_i-1)} e^{-r_i/2} e^{-\alpha(R_o+\sum_i R_i r_i/\nu_i)}}{R_o+\sum_i R_i/\nu_i} \tag{M.7}$$

so that,

$$J = I\ (0).$$

Evaluation of $\frac{dI}{d\alpha}$ is easily done due to the cancellation of the denominator in (M.7) yielding the result:

$$-\frac{dI}{d\alpha} = e^{-\alpha R_o} \prod_i^n \frac{2^{(\nu_i+2m_i)/2}\Gamma(m_i+\nu_i/2)}{(1+2R_i\alpha/\nu_i)^{(2m_i+\nu_i)/2}} \tag{M.9}$$

Integration of (M.9) together with the use of (M.7) and (M.8) then yields:

$$J = \prod_{i=1}^{n}\left[2^{(m_i+\nu_i/2)}\ \Gamma(m_i+\nu_i/2)\right]\int_0^\infty e^{-\alpha R_o} \prod_{i=1}^{n} (1+2R_i\alpha/\nu_i)^{-(m_i+\nu_i/2)} d\alpha \tag{M.10}$$

It follows from (M.5) and (M.10) that:

$$\left\langle \frac{\Gamma_i \Gamma_n}{\Gamma} \right\rangle = \frac{\overline{\Gamma}_i \overline{\Gamma}_n}{\overline{\Gamma}\nu_i \nu_n} \prod_{i=1}^{n} 2^{m_i}\Gamma(m_i+\nu_i/2)/\Gamma(\nu_i/2)\ H, \tag{M.11}$$

where:

$$H = \int_0^\infty d\alpha \; e^{-\alpha R_o} \prod_{i=1}^{n} (1+2R_i\alpha/\nu_i)^{-(m_i+\nu_i/2)} . \tag{M.12}$$

Here $m_i = 0$, 1 or 2 depending on whether reaction width Γ_i appears as a factor zero, once, or twice, respectively, in the numerator of the left hand side of (M.11).

M.2 Numerical Evaluation of the Cross Section by Gaussian Quadrature

In order to evaluate the integral H we first make the substitution:

$$\alpha = \frac{1-\mu}{1+\mu} \quad , \quad -1 \le \mu \le +1 \tag{M.13}$$

This results in the following expression:

$$H = 2 \int_{-1}^{+1} (1+\mu)^{-2} \prod_i \left[1+\frac{2R_i}{\nu_i}\,\frac{1-\mu}{1+\mu}\right]^{(m_i+\nu_i/2)} \exp(-R_o \frac{1-\mu}{1-\mu}) d\mu \tag{M.14}$$

In all practical cases the value of the integrand rises sharply from zero at $\mu=-1$ and contains no singularities in the entire interval -1 to +1. The method of Gaussian integration over this interval with the zeros of the Legendre Polynomial of order ℓ taken as points of tabulation should then yield a rapid scheme of integration.

A check on the accuracy of the integration scheme is easily made. Note that:

$$\sum_i \left\langle \frac{\Gamma_n \Gamma_i}{\Gamma} \right\rangle = \bar{\Gamma}_n , \tag{M.15}$$

which can be compared with the sum of the integrals for all reactions.

Actual experience with the Gaussian integration has shown that 20 points yield fractional errors of about 5×10^{-5} in the Γ_n comparison, while 10 points has an associated error of 2×10^{-3}. Use of 20 points in the integration scheme is fully satisfactory and has been implemented in the code. Table M.1 presents the abscissas, μ, and the weights used in the 20 point integration scheme. These values are taken from reference 1, Table 25.4.

Table M.1 - Abscissas and Weight Factors for Gaussian Integration

Point Number	Abscissa	Weight
1	-0.99312860	0.0176149
2	-0.96397193	0.04060143
3	-0.91223443	0.06267205
4	-0.83911697	0.08327674
5	-0.74633191	0.10193012
6	-0.63605368	0.11819453
7	-0.51086700	0.13168864
8	-0.37370609	0.14209611
9	-0.22778585	0.14917299
10	-0.07652652	0.15275339
11	+0.07652652	0.15275339
12	+0.22778585	0.14917299
13	_0.37370609	0.14209611
14	+0.51086700	0.13168864
15	+0.63605368	0.11819453
16	+0.74633191	0.10193012
17	+0.83911697	0.08327674
18	+0.91223443	0.06267205
19	+0.96397193	0.04060143
20	+0.99312860	0.01761401

REFERENCE FOR APPENDIX M

1. M. Abramowitz and I.A. Stegun, Editors, "Handbook of Mathematical Functions", National Bureau of Standards Publication, Library of Congress Catalog Card Number; 64-60036 (1964).

APPENDIX N

Structure of the BCD Element Data Tape (EDT)*

Each record of the BCD EDT is a sequenced, 80 column card image (see Figure N.1). The sequence number, singly incremented, is right-adjusted in columns 76-80. Columns 71-75 display the assigned MAT #. The last record for a material is signaled by a negative MAT #. The bulk of the data, entered in columns 1-70 of each record, comprises 4 or 6 contiguous groups of records, as described below.

Group 1: Records 1 and 2

Record #1 (I14, E14.6, 3I14)

Item	Columns	Variable	Description
1	1-14	LENGTH	Total number of entries on the corresponding binary EDT for this material.
2	15-28	ATWT	Atomic weight
3	29-42	ID	Element Identifier
4	43-56	NREC	One less than total number of BCD records for this material.
5	57-70	KCNT	Number of entries (binary EDT) prior to second floating point word (first is ATWT).

Record #2 (5I14)

Item	Columns	Variable	Description
1	1-14	IT	Number of text records.
2	15-28	IRECA	Number of records in Group 3.
3	29-42	NEG	Number of photon energies (GPDT) or levels (NEDT).
4	43-56	IRECC	Number of records in Group 5, if NEG>0; ignored if NEG = 0.
5	57-70	IRECD	Number of records in Group 6.

*Familiarity with Appendices A, B, and D is a prerequisite for a full understanding of this Appendix.

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```
      177   9.991700E-01          1001            39           59 4148    1
        1             12            17             4           17 4148    2
HYDROGEN GFDT MAY 1972.                                            4148    3
     1001             93            34             8            0 4148    4
       17            127           129           132          135 4148    5
      138            141           144           147          150 4148    6
      153            156           159           162          165 4148    7
      168            171           174            33           34 4148    8
       31             33            29            31           27 4148    9
       29             25            27            23           25 4148   10
       21             23            19            21           17 4148   11
       19             15            17            13           15 4148   12
       11             13             9            11            7 4148   13
        9              5             7             3            5 4148   14
        1              3             7             3            5 4148   15
2.225000E 06  2.425000E 06  2.625000E 06  2.975000E 06  3.475000E 06 4148   16
3.975000E 06  4.475000E 06  4.975000E 06  5.475000E 06  5.975000E 06 4148   17
6.475000E 06  6.975000E 06  7.725000E 06  8.725000E 06  9.725000E 06 4148   18
1.072500E 07  1.172500E 07  7.725000E 06  8.725000E 06  9.725000E 06 4148   19
        0              0             0             0            0 4148   20
        0              0             0             0            0 4148   21
        0              0             0             0            0 4148   22
        0              0             0             0            0 4148   23
2.000000E 07  1.850000E 07  1.800000E 07  1.650000E 07  1.600000E 07 4148   24
1.450000E 07  1.400000E 07  1.250000E 07  1.200000E 07  1.050000E 07 4148   25
1.000000E 07  9.500000E 06  9.000000E 06  8.500000E 06  8.000000E 06 4148   26
7.500000E 06  7.000000E 06  6.200000E 06  6.000000E 06  5.200000E 06 4148   27
5.000000E 06  4.200000E 06  4.000000E 06  3.200000E 06  3.000000E 06 4148   28
2.200000E 06  2.000000E 06  1.100000E 06  1.000000E 06  6.500000E 05 4148   29
6.000000E 05  2.200000E 05  2.000000E 05  1.000000E-05  1.000000E 00 4148   30
1.000000E 00  1.000000E 00  1.000000E 00  0.            1.000000E 00 4148   31
1.000000E 00  0.            1.000000E 00  1.000000E 00  0.           4148   32
1.000000E 00  1.000000E 00  0.            1.000000E 00  1.000000E 00 4148   33
0.            1.000000E 00  1.000000E 00  0.            1.000000E 00 4148   34
1.000000E 00  0.            1.000000E 00  1.000000E 00  0.           4148   35
1.000000E 00  1.000000E 00  0.            1.000000E 00  1.000000E 00 4148   36
0.            1.000000E 00  1.000000E 00  0.            1.000000E 00 4148   37
1.000000E 00  0.            1.000000E 00  1.000000E 00  0.           4148   38
1.000000E 00  1.000000E 00  0.            1.000000E 00  1.000000E 00 4148   39
0.            1.000000E 00  1.000000E 00  0.            1.000000E 00-4148   40
```

FIGURE N.1. A Sample BCD EDT.

Group 2: IT Hollerith Records

The format (17A4, A2) is repeated for IT records of descriptive text.

Group 3: IRECA Fixed Point Records

The format (5I14) is repeated for IRECA records of pointers. If the number of pointers is not a multiple of 5, the remaining entries on the last record in this group repeat the corresponding entries on the next to last record (there are always more than one record for both an NEDT and a GPDT).

Group 4: Discrete Energy Records

If NEG=0, this group is omitted. For NEG>0, the format (5E14.6) is repeated for IRECB (=(NEG-1)/5+1) records of either photon energies, in the case of a GPDT, or level excitations, in the case of an NEDT. If NEG is not a multiple of 5, the remaining entries on the last record in this group repeat the corresponding entries on the preceding record.

Group 5: IRECC Fixed Point Records

If NEG=0, this group is omitted. For NEG>0, the format (5I14) is repeated for IRECC records of remaining pointers. The last record may be filled-in, as above.

Group 6: IRECD Floating Point Records

The format (5E14.6) is repeated for IRECD records of floating point data beyond the pointers, i.e., energy table and yields for a GPDT, or energy tables, cross sections, and distribution tables for an NEDT. The last record, signaled by a negative MAT in columns 71-75, may include a few fill-in entries, as described above.

APPENDIX O

Bounded Flux-At-A-Point (BFAP) Estimation

1. Introduction

In many instances, the availability of a point estimation capability represents a desirable extension of the ordinary track length, or volume estimation method. However, unless special biasing procedures are employed, flux-at-a-point estimation effects infinite variance.

A very efficient scheme, developed by Steinberg and Kalos[1], involves biased selection of source and collision points such that, not only are subsequent "last flight" estimates at point detectors made with finite variance, but, in addition, all estimates are made with a finite upper bound. This combination of biased selection and "last flight" estimation, the so-called bounded flux-at-a-point (BFAP) estimation, is superior to the so-called "once-more-collided" flux-at-a-point (FAP) estimation because fewer histories are required to achieve a given statistical accuracy.

The sections which follow describe the mathematical basis for, and the coding implementation of the algorithms comprising the BFAP estimation procedure.

2. Theory

2.1 Point Estimation

The following procedure can be used to make flux-at-a-point estimates. In the course of each Monte Carlo history, at the time

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of position (source or collision) selection, a virtual ray is traced from the selected position to the detector. The estimator term, f, is given by the expression (where Ω is the direction vector of the virtual ray):

$$f = Wg(\Omega)\exp(-\int\sigma(s)ds)/4\pi R^2$$

where W is the particle weight at the selected position, $g(\Omega)$ is the differential directional distribution (discussed below), σ is the total macroscopic cross-section, and R is the distance between the selected position and the detector. The integration in the exponential is along the straight line path from the selected position to the detector.

The term $g(\Omega)$ out of a source would be constant for isotropic distributions; otherwise it is a prescribed function of direction. At a collision, the situation is more complicated. The collision procedure is usually carried out in several selection steps: (1) position, (2) target element, (3) reaction process, (4) scattering angle. The most efficient place to carry out the point estimation is between steps (3) and (4), where W reflects the state of the particle after step (3). $g(\Omega)$ is then, simply, the (laboratory) angular distribution of the selected reaction for the selected target, and is actually a function of $\Omega_o \cdot \Omega$, where Ω_o is the particle direction entering collision.

The principal problem associated with such an estimation procedure is the presence of the R^2 term in the denominator of f. If the selected position is near the detector, the estimator is arbitrarily large in value. As a means of overcoming this problem, Steinberg and Kalos devised a procedure (discussed below) where the position selection is biased so that W contains a compensating factor proportional to R^2. This then leads to an upper bound for f.

2.2 Bounded Estimation

Since a full discussion of the theory of bounded estimation for point detectors is given in Reference 1, only the essentials will be described. Consider a region around the detector at x_D (e.g., a sphere of radius R_o centered at the detector, or a region of some other shape containing such a sphere). Then, if the position selection is biased to be approximately uniform in the distance from the detector, the compensating weight factor contains a term proportional to R^2, where R is the distance between the detector and the selected position.

When the selected position x is a collision position, care must be taken that the distance to the previous particle position x_o is also biased properly to avoid a singularity of the form R_1^{-2}, where R_1 is the distance between the previous position and the collision position. This can be accomplished by first biasing the direction out of the previous collision so that selection of the angle α between $(x-x_o)$ and (x_D-x_o) is proportional to α rather than the "natural" $\cos\alpha$ (ignoring local anisotropy). Then the position along the path is selected from a probability density with a factor $1/R^2$.

In Reference 1, an implementation using a reselection procedure was described, where x is reselected within the detector region by reselecting α and the distance along the ray. (If the selected position is a source position, the problem does not exist, and the method described in Reference 1 applies.) The principal drawback of this procedure is the need for the availability of the angular distribution data to get the proper weight adjustment for the selection. If the previous position was also a collision, this

angular distribution data is a function of the particle energy before the previous collision, which might not be available at the time the reselection takes place, because a different band of cross section data is in the machine.

To avoid this programming difficulty, the angle portion of the biasing is carried out concurrently with the selection of the direction out of the previous position. The biasing of the distance along the ray is carried out later in the course of selecting the collision position.

2.3 Multiple Detectors

In general, the procedures described above can be easily implemented when there are several point detectors. The estimation procedure becomes, essentially, a repetition of the single detector scheme, with the added complication of possible interactions between the detectors. The algorithms utilized to resolve this multi-detector complication are discussed in Section 4.

3. Code Implementation

The implementation of BFAP estimation comprises several distinct aspects: (1) problem initialization; (2) angle reselection; (3) position selection; and (4) resolution of multiple detector conflicts. The first three aspects are discussed in Sections 3.1 to 3.3. Multiple detector effects are the subject of Section 4.

3.1 Problem Initialization

After reading in user supplied information about the point detectors, two basic characteristics are precomputed for each detector. The first characteristic is the so-called "critical radius", which defines a sphere of influence about the detector point, also referred to as the "critical sphere." The algorithm for computing this radius is

$$R_k = (\bar{u}_k)^{-1} \qquad (0\text{-}1)$$

where $\bar{u}_k$ is the total macroscopic cross section of the material region designated for the k-th detector, evaluated for a nominal microscopic cross section of 1 barn/atom.

The second characteristic determined for each detector is a "critical sphere overlap" flag, which is utilized in the resolution of multiple detector conflicts. If $\{x_k\}$ are the detector locations, then the algorithm for determining $\{L_k\}$ (initialized to 0) is

$$|x_k - x_i|^2 < (R_k + R_i)^2, \text{ for any } i \neq k; \text{ set } L_k = 1 \qquad (0\text{-}2)$$

3.2 Angle Reselection

Angle reselection is indicated whenever an originally selected (OS) ray intersects the critical sphere of a live detector. In addition, for post scattering (as opposed to source) directions, the corresponding post scattering energy must be recomputed. Furthermore, for near threshold inelastic or hydrogen scattering of neutrons, for which the effective mass of recoiling nucleus is $A' \leq 1$ [neutron mass], a special treatment is required, since a range of scattered directions becomes physically impossible.

3.2.1 Angle Reselection (General)

Let W be the originally selected (OS) direction. The algorithm for determining the intersection of live critical spheres proceeds as follows: For each live detector, let $W_k = (x_k - x)/|x_k - x|$, where x_k is the position of the k-th detector, and x is the particle position. Let $\delta_k = W \cdot W_k$. Then, if

$$\delta_k^2 > 1 - R_k^2/|x - x_k|^2, \quad (\delta_k > 0) \tag{O-3}$$

the k-th critical sphere is intersected by the OS ray. If no live detector satisfies the conditions of (O-3), no reselection is necessary, and the remaining procedure is bypassed. If more than one live detector sphere is intersected by the OS ray, a "multiple detector conflict" (MDC) exists. Even if only one detector sphere is intersected, an MDC may have to be resolved due to sphere or cone overlap (see Section 4).

Ultimately, subsequent to possible resolution of an original MDC, at most one live detector sphere, k, will be intersected by the OS ray. The angle reselection, then, proceeds as follows: choose an angle θ^* uniformly in the range $[\theta_H, \theta_L]$ given by

$$r = \min\{R_k/|x - x_k|, 1.0\} \tag{O-4a}$$

$$\theta_H = \sin^{-1}(r) \tag{O-4b}$$

$$\theta_L = -\theta_H \tag{O-4c}$$

For near threshold inelastic or hydrogen scattering, the algorithm of (O-4) is replaced by the special procedure described in the next section.

The reselected angle θ^* yields a reselected (RS) direction (or ray) W^* given by

$$W^* = \alpha W + \beta W_k \tag{O-5a}$$

where

$$\alpha = \sin \theta^* / \sin \theta \tag{O-5b}$$

$$\beta = \sin (\theta - \theta^*) / \sin \theta \tag{O-5c}$$

$$\theta = \cos^{-1} (W \cdot W_k) \tag{O-5d}$$

To avoid the singularity when $\theta = 0$, the following algorithm precedes (O-5): Let $W = W_k = (v_1, v_2, v_3)$. Find i for which $|v_i|$ is smallest. Let new W be the vector formed by adding 0.01 to the i-th component of W_k, and normalizing to unity.

Finally, the particle weight must be adjusted by a factor

$$W_a = C\, q(\Delta^*)/q(\Delta) \tag{O-6a}$$

where q is the sampling density for lab angle cosines (Δ and Δ^* are the OS and RS values, respectively), and

$$C = |\sin \theta^*| \ (\theta_H - \theta_L)/I(\theta_H, \theta_L) \tag{O-6b}$$

$$\begin{aligned} I(\theta_H, \theta_L) &= \cos\theta_L - \cos\theta_H, \ \theta_L \geq 0 \\ &= 2 - \cos\theta_H - \cos\theta_L, \theta_L < 0 \end{aligned} \tag{O-6c}$$

3.2.2 Special Procedure For $A' \leq 1$ Case

For near threshold inelastic and hydrogen scattering, where the (effective) weight of the recoiling nucleus $A' \leq 1$, the general algorithms (O-3) and (O-4) are modified as follows: in addition to the constraint of (O-3), the condition:

$$W \cdot W_k < W_o \cdot W_k \tag{O-7}$$

effects a bypass of angular reselection, where W_o, W, and W_k are the pre-scattering, OS, and the direction to the k-th detector, respectively.

If (O-7) is not satisfied, the special procedure for $A' \leq 1$ proceeds with the computation of three angles β, δ, γ in the range $(0, \pi)$.

$$\beta = \sin^{-1}(A'); \qquad 0 \leq \beta \leq \pi/2 \qquad \text{(O-7a)}$$

$$\delta = \cos^{-1}(W_k \cdot W_o) \qquad \text{(O-7b)}$$

$$\gamma = \min(\delta, \theta_H) \qquad \text{(O-7c)}$$

where θ_H is given by (O-4b).

If $\beta \geq \gamma + \delta$, the remainder of the special procedure is bypassed. Otherwise, define $\psi_M = \frac{\pi}{2}$, $(\beta > \delta)$;

$$= \cos^{-1}\left[(\cos\beta - \cos\delta\cos\gamma)/(\sin\delta\sin\gamma)\right] (\beta \leq \delta) \qquad \text{(O-8)}$$

Choose ψ uniformly in $\left[0, \psi_M\right]$. Compute a temporary W, as input to the reselection, using

$$W = A\, W_k + B\, W_o + C\, (W_k \times W_o) \qquad \text{(O-9)}$$

where

$$A = \cos\delta(1 - \cos\psi) \qquad \text{(O-10a)}$$

$$B = \cos\psi \qquad \text{(O-10b)}$$

$$C = \pm \sin\psi \qquad \text{(O-10c)}$$

The sign of C is chosen at random with equal probability.

As a final preparation to the reselection procedure, it is necessary to define θ_H, θ_L, and θ. Substituting (O-9) into (O-5d) yields $\theta = \delta$.

Let $$U = \cos\psi\sin\delta \qquad \text{(O-11a)}$$

$$V = \sqrt{\sin^2\beta - \sin^2\psi\sin^2\delta} \qquad \text{(O-11b)}$$

$$X = \cos^2\psi\sin^2\delta + \cos^2\delta \qquad \text{(O-11c)}$$

Define $\theta_{\pm}$ in the range $(0,2\pi)$ using:

$$\cos\theta_{\pm} = (\cos\beta\cos\delta \pm UV)/X; \quad \psi < \pi/2 \tag{O-12a}$$

$$\sin\theta_{\pm} = \frac{\cos\beta - \cos\delta\cos\theta_{\pm}}{\sin\delta\cos\psi}; \quad \psi < \pi/2 \tag{O-12b}$$

$$\cos\theta_{\pm} = \cos\beta/\cos\delta \ ; \ \psi = \pi/2 \tag{O-12c}$$

$$\sin\theta_{\pm} = \pm\sqrt{1 - \cos^2\theta_{\pm}} \ ; \ \psi = \pi/2 \tag{O-12d}$$

Then, using $\theta_{\pm}$ as defined above:

$$\theta_1 = \max(\theta_+, \theta_-) \ ; \quad \beta \le \delta \tag{O-13a}$$

$$\theta_2 = \min(\theta_+, \theta_-) \ ; \quad \beta \le \delta \tag{O-13b}$$

$$\theta_1 = \min(\theta_+, \theta_-) \ ; \quad \beta > \delta \tag{O-13c}$$

$$\theta_2 = \max(\theta_+, \theta_-) - 2\pi \ ; \ \beta > \delta \tag{O-13d}$$

$$\theta_H = \min(\theta_1, \gamma) \tag{O-13e}$$

$$\theta_L = \max(\theta_2, -\gamma) \tag{O-13f}$$

An additional weight adjustment factor C must be computed by:

$$C = \frac{\psi_M I(\theta_H,\theta_L)}{\pi - \Omega - \eta\cos\beta - \psi_M\cos\gamma}$$

where $I(\theta_H,\theta_L)$ is given by (O-6c). Ω and η are angles between 0 and π, given by:

$$\eta = \cos^{-1}((\cos\gamma - \cos\beta\cos\delta)/\sin\beta\sin\delta) \tag{O-14a}$$

$$\Omega = \cos^{-1}((\cos\delta - \cos\beta\cos\gamma)/\sin\beta\sin\gamma) \tag{O-14b}$$

3.3 Position Reselection

By means of the algorithms (discussed in Section 4) designed to resolve an MDC, it is possible for the particle ray to intersect only one sphere of radius R_k centered at a live detector (see Figure 0.1).

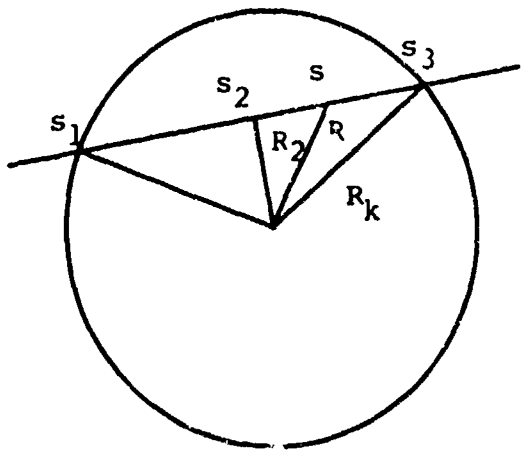


Figure 0.1

If a collision falls between s_1 and s_2, reselect in that interval; similarly for a collision between s_2 and s_3. The exact density $f(s)$ for reselection can be written as:

$$f(s) = g(s) \Big/ \int_{s_i}^{s_{i+1}} g(t)dt \tag{O-15}$$

where

$$g(s) = \mu(s)W(s)e^{-\int_{s_i}^{s} \mu(t)dt} \Big/ \left[(s-s_2)^2+R_o^2\right] \tag{O-16}$$

and W(s) is the importance (sampling) weight at s. Since the exact integration of g(s) is very difficult, it suffices to use an approximation to g(s) as shown below.

Track from s_2 to either s_1 or s_3. Define $t_o = s_2$. Generate t_i sequentially as the minimum of .5 mean free path distance or a region boundary crossing until s_1 or s_3 is reached, which then becomes t_n.

For each interval, define Q_i by:

$$Q_i = W_i \mu_i \, B_i \, \left(\arctan\left(\frac{|t_i - t_o|}{R_o}\right) - \arctan\left(\frac{|t_{i-1} - t_o|}{R_o}\right)\right) \tag{O-17}$$

where W_i is importance weight, and μ_i is cross section, while $B_i = (A_i + A_{i-1})$ and A_i is defined recursively (with A_o=1) by:

$$A_i = A_{i-1} \exp\left(-\mu_i (t_i - t_{i-1})\right) \tag{O-18}$$

Note that when tracking from s_2 to s_1 (backwards) the A_i increase with i.

To reselect a point, first choose an interval $I_i = (t_{i-1}, t_i)$ with probability $P_i = Q_i / \Sigma Q_j$. Then select a point t within the interval I_i using the formula below:

$$|t-t_o| = R_o \tan\left(\xi \arctan\left(\frac{|t_i-t_o|}{R_o}\right) + (1-\xi)\arctan\left(\frac{|t_{i-1}-t_o|}{R_o}\right)\right) \tag{O-19}$$

where ξ is a random number.

Finally the carry along weight of the particle must be multiplied by C given by:

$$C = \left\{(R_o^2 + (t-t_o)^2)\right\} \frac{\Sigma Q_j}{B_i} \; \frac{\exp\left(-\int_{s_k}^{t} \mu(p)\,dp\right)}{\int_{s_k}^{s_{k+1}} \mu(p) W(p) \exp\left(\int_{s_k}^{p} \mu(q)\,dq\right) dp} \tag{O-20}$$

4. Multiple Detector Conflicts (MDC)

4.1 Introduction

Since the special biasing schemes of the BFAP estimation procedure are based on the concept of detector spheres of influence, the simultaneous presence of several detectors defines potentially overlapping regions of influence. Such regions represent multiple detector conflicts (MDC). The MDC are resolved via the "live detector" concept described in the sections that follow.

4.2 The MDC Condition

Relevant to the aspect of angle reselection, the MDC condition exists whenever any pair of live detectors satisfies the "cone overlap test" (COT): let X, X_k, and X_ℓ, be the positions of the particle, and the k-th, and the ℓ-th detector, respectively. Let $\beta_{k\ell} = W_k \cdot W_\ell$, where $W_k = (X_k-X)/|X_k-X|$, and W_ℓ is similarly defined. Then, if

$$\beta_{k\ell} \geq \sqrt{\left(1 - \frac{R_k^2}{|X-X_k|^2}\right)\left(1 - \frac{R_\ell^2}{|X-X_\ell|^2}\right)} - \frac{R_k R_\ell}{|X-X_k|\,|X-X_\ell|}$$

the COT is satisfied, and an MDC exists.

Although references to "sphere overlaps" (see algorithm (O-2)) and "multiple intersections" (see algorithm (O-3)) also imply the existence of an "angle" MDC, these tests comprise a sub-set of the COT. Finally, only a sphere overlap is a significant MDC for position reselection.

4.3 Resolution of an MDC

An MDC may be resolved by Russian roulette, in which one ("live") detector is chosen for sampling purposes. The implication of this selection depends on the particular stage of the particle history at which it occurs.

4.3.1 Position Checking (Source)

After the selection of a source position at the start of a history, the resolution of an MDC is recorded by the appropriate setting of the live detector "position flag", KDLIV. The relevant algorithms are best summarized by a logical flow chart (Figure 0-2).

The case KDLIV ≥ 0 implies that there was no MDC. For KDLIV<0 detector #-KDLIV is used for sampling purposes and a special weight adjustment [2] is necessary to permit bounded estimation for all detectors. (See below.) Furthermore, the value of KDLIV influences the direction checking that precedes angle reselection, as described in Section 3.2. The special weight adjustment is $nb_k / \sum_{m=1}^{n} b_m$, where $k=|\text{KDLIV}|$, and $b_m=\max(1, R_m^2/|X-X_m|^2)$.

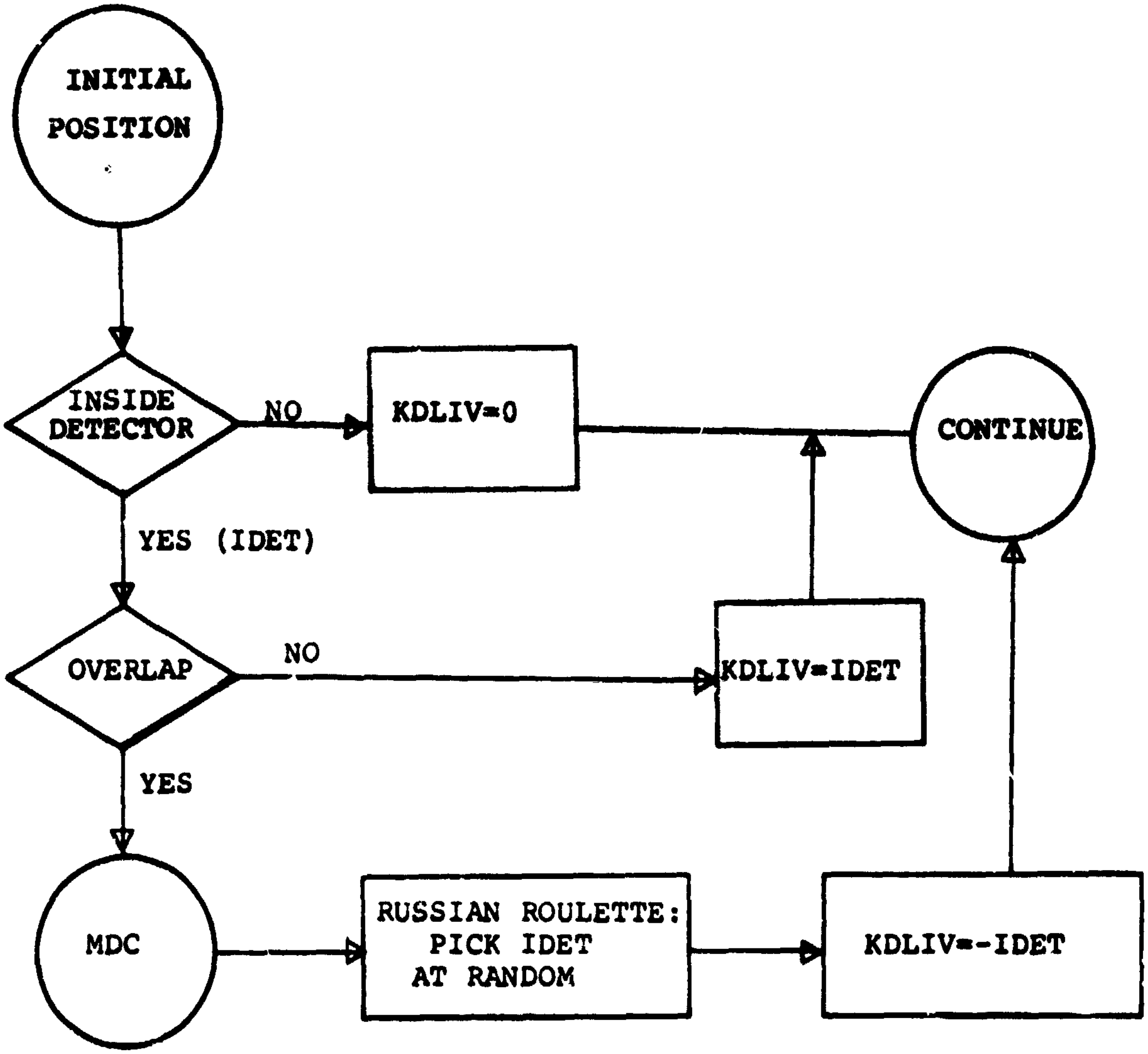


Figure O.2

4.3.2 Direction Checking

Subsequent to position checking (both at a source and a collision* point), there are a series of direction checks aimed at resolving an angle MDC by appropriate setting of a live detector "direction flag," NDLIV. In order to distinguish between a latent and the current ray being tracked, another "direction flag," IDLIV assumes the role and the value of (the computed) NDLIV, whenever a source particle or latent is picked up for tracking.

* Refer to Section 4.3.3 of this Appendix.

As in the setting of KDLIV, the relevant algorithms for computing NDLIV are best summarized by a logical flow chart.

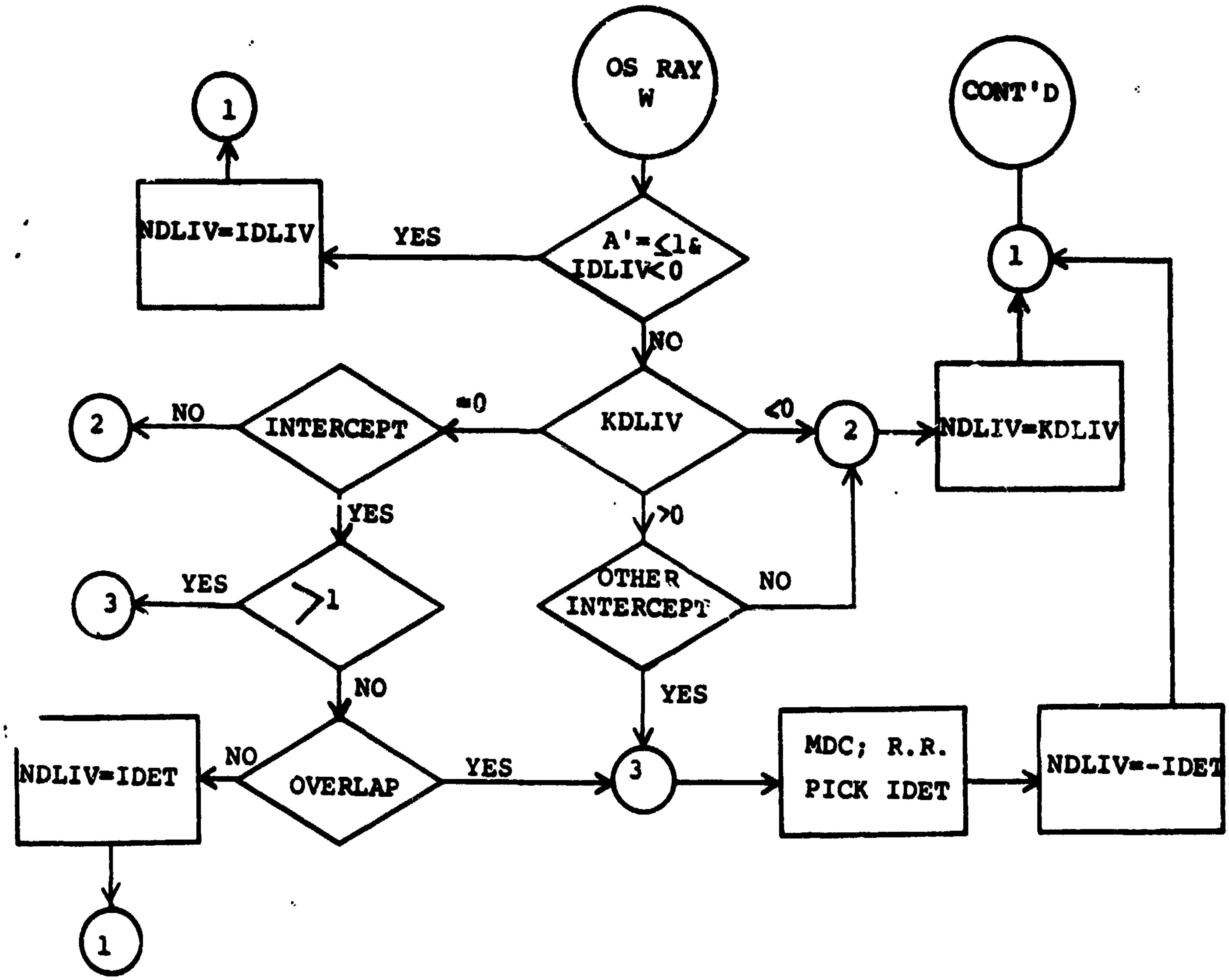


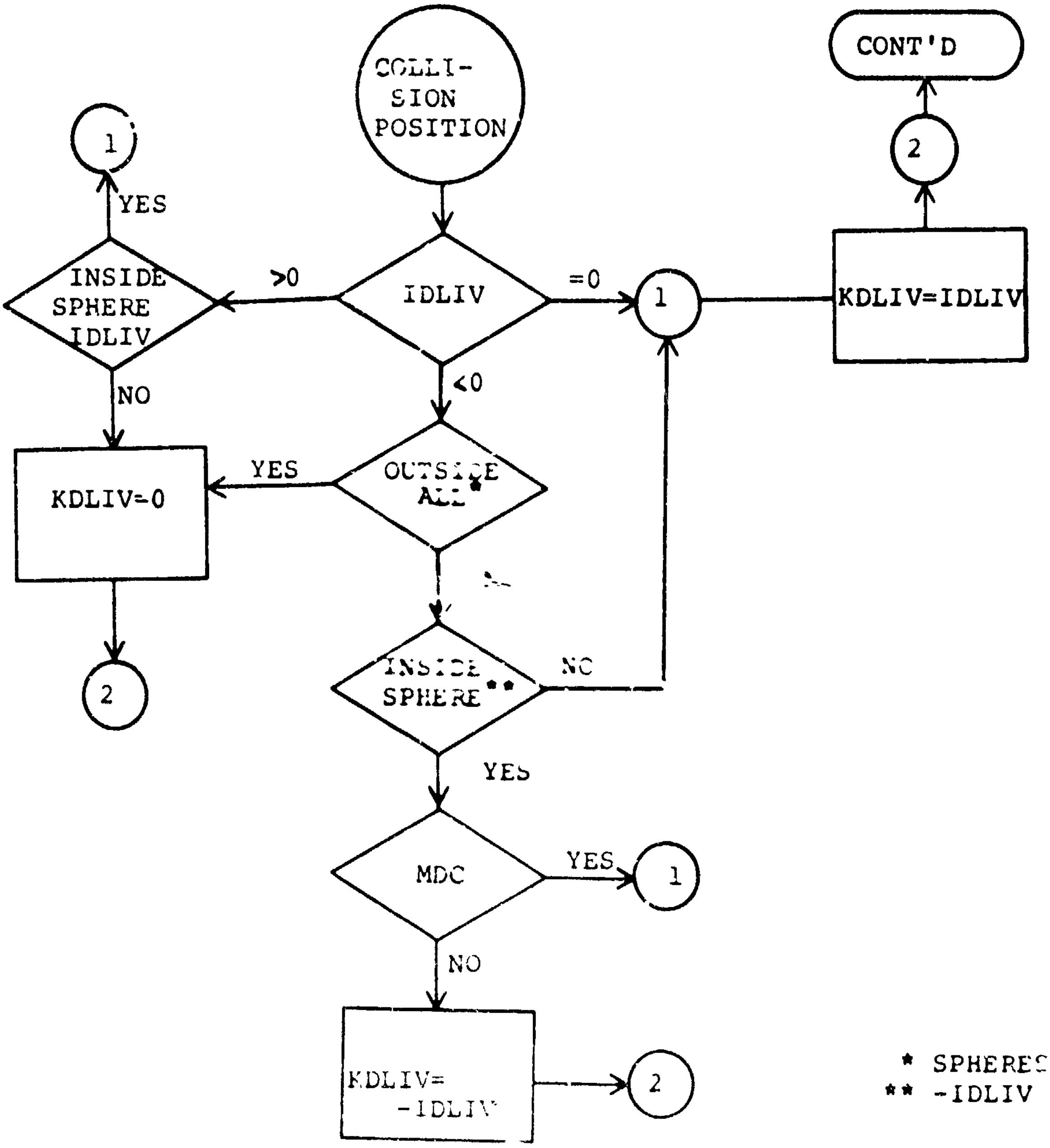
Figure 0.3

By means of the IDLIV (NDLIV) definition, sampling along the particle ray can be affected by at most one sphere of radius R_k centered at a detector. Thus, for IDLIV>0, detector sphere #IDLIV is used; for IDLIV=0, no spheres are used; and for IDLIV<0, #-IDLIV is used for sampling and the special weight adjustment is carried out.

The value of IDLIV also influences the position checking at a collision point, as described in the next section.

4.3.3 Position Checking (Collision)

Subsequent to the selection of a collision point along the current ray, which is characterized by IDLIV (as opposed to NDLIV, which is computed for a latent), a value of KDLIV is computed for the latent to be stored. This value of KDLIV has the same significance for the latent as the KDLIV which is computed for the source position. Again, the position checking algorithms at the collision are best summarized by the corresponding flow chart:



REFERENCE FOR APPENDIX O

1. H.A. Steinberg and M.H. Kalos, Nuc. Sci. and Eng., 44, 406-412 (1971).

2. H. A. Steinberg, Bounded Estimation of Flux-at-a-Point for One or More Detectors, ANL-NEACRP Meeting of a Monte Carlo Study Group, Argonne National Lab., July 1974.

APPENDIX P

Combinatorial Geometry Example Employing All Allowed Body Types

The data sheets which follow, provide the complete input description for Combinatorial Geometry Example #5, as shown in Section 3.2.1.3.

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FORTRAN STATEMENT

SPECIAL INSTRUCTIONS

card code = 026
029

0 = ZERO 1 = ONE 2 = TWO
Ø = ALPHA O I = ALPHA I Z = ALPHA Z

STATEMENT NO								IDENTIFICATION
	0	0	0	1.	EXAMPLE EMPLØYING ALL ALLØWED BØDY TYPES			
RPP	1	-12.	12.	-12.	12.	-16.	18.	
BØX	2	-11.	-11.	-12.	20.	0.	0.	
		0.	20.	0.	0.	0.	28.	
TRC	3	0.	0.	-10.	0.	0.	24.	
		4.	8.					
REC	4	0.	0.	13.	0.	0.	2.5	
		4.	0.	0.	0.	3.	0.	
ARB	5	-6.	-5.	12.	-5.	-5.	2.	
		5.	-5.	1.	5.	-5.	12.	
		5.	5.	1.	5.	5.	12.	
		-6.	5.	12.	-5.	5.	2.	
		2341.	3564.	8765.	2178.	1467.	3285.	
RAW	6	-5.	-5.	1.	0.	0.	1.	
		10.	0.	0.	0.	10.	0.	
RCC	7	-8.5	0.	-9.	0.	0.	5.	
		1.5						
ELL	8	8.	0.	-9.3	8.	0.	-5.7	
SPH	9	-.5	0.	-11.5	2.			

(continued on next page)

FORTRAN STATEMENT

STATEMENT NO	CONT				SPECIAL INSTRUCTIONS	IDENTIFICATION
		0 = ZERO	1 = ONE	2 = TWO	card code = 026 029	
		Ø = ALPHA O	I = ALPHA I	Ƶ = ALPHA Z		

```
TEC    10   -1.        0.        -1.       1.5       0.        1.
             0.        0.         1.       1.        0.        0.
             1.        0.75       2.
END
1                 1    -2
2                 2    -3    -4    -5    -6    -7    -8    -9
3        ØR       3    -5    -6    -10ØR  4
4                 5    -6
5                 6
6                 7    -9
7                 8
8                 9    -2    -7
9                 7     9
10               10
END
```

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APPENDIX Q

Selection of Collision Positions from the Importance Biased Transport Kernel

Let $W(\vec{X},E,\vec{\Omega})$ be the importance weight factor of a particle at position $\vec{X}$ flying in direction $\vec{\Omega}$ at energy E. If a particle is born at position $\vec{X}'$, in direction $\vec{\Omega}$ at energy E, the density of its collisions at a distance S along the track is given by

$$F(s)ds = F\frac{W(\vec{X}',E\vec{\Omega})}{W(X'+s\vec{\Omega},E\vec{\Omega})}\ \mu(\vec{X}'+s\vec{\Omega},E),$$

$$\exp\left[-\int_0^s \mu(\vec{X}'+s'\vec{\Omega},E)ds'\right] ds$$

Further modifications of the above distribution may occur if point detectors are used. The modifications are then confined to that part of the track which is within a prescribed cutoff distance from one of the point detectors. This case is not covered here, but its discussion is given in Section 3.3 of Appendix O.

The distribution F(s)ds is not, in general, a probability distribution function, as it is not necessarily normalized to unity. The unbiased transport kernel

$$\mu\ \exp\left(-\int_0^s \mu ds\right)$$

is normalized to unity. But the biasing function

$$F\frac{W(X',E\vec{\Omega})}{W(X'+s\vec{\Omega},E\vec{\Omega})}$$

in general destroys that normalization.

Figure Q.1a shows a schematic plot of the function F(s), drawn under the assumption that $\vec{\Omega}$ points into a direction of increasing importance (i.e., of decreasing weights). As can be seen, the s-dependence is $e^{-\mu s}$ in each region, with a discontinuity at each boundary where a change in weight and(or) of μ occurs.

To pick s from such a distribution, we construct the function:

$$G(s) = \int_0^s F(s)\, ds$$

$G(\infty)$ gives the normalization of F(s).

If N is an integer such that $N \leq G(\infty) < N + 1$, we will arrange to pick either N or N + 1 distances s, with probability $[N + 1 - G(\infty)]$ or $[G(\infty) - N]$, respectively. Furthermore, the collision points will be picked in a stratified way.

To pick the first collision point, we pick a random number ξ_1 and solve (see Figure Q.1b)

$$G(s_1) = \xi_1.$$

To pick the second collision point, we pick another random number ξ_2 and solve

$$G(s_2) = 1 + \xi_2, \text{ etc.}$$

Before solving for each s_n, $n=1, \ldots, n+1$, $G(s_n) = n - 1 + \xi_n$, we test whether such a solution exists, i.e., whether $G(\infty)\ n - 1 + \xi_n$. If the test is not passed, no n^{th} and no further collisions should be generated from that flight.

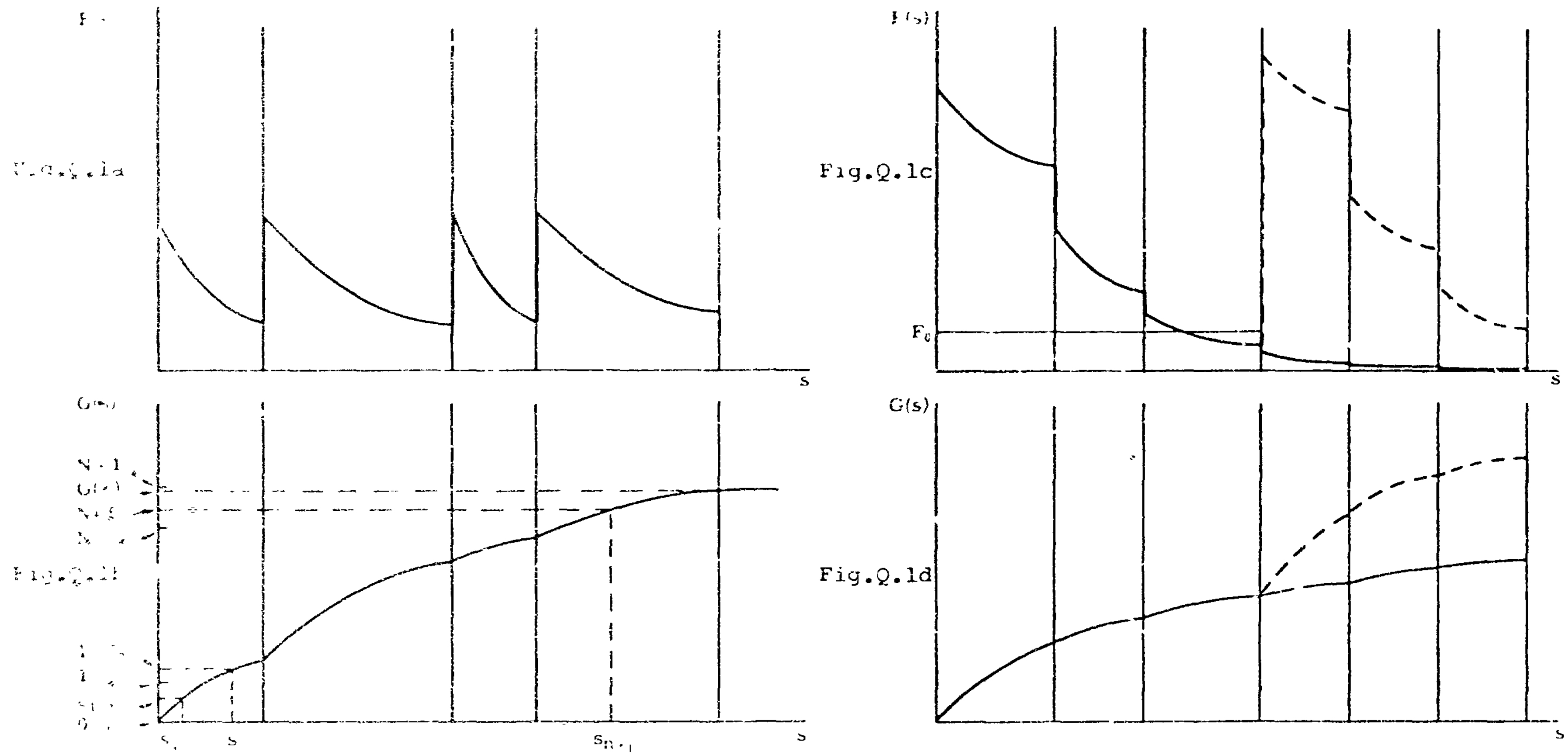


Fig. Q.1 – Schematic Diagram of the s-Dependence of the Modified Transport Kernel F(s) and of the Integral

$$G(s) = \int_0^s F(s)\,ds$$

Actually, we do not pick n different random numbers, but just a single one at the beginning of the flight, and set $\xi_2 = \xi_3 = \ldots. = \xi_n = \xi_1$.

In the actual coding, the tracking, integration, and selection of collision points are done simultaneously.

In describing the process, it is implied that we always have to track to ∞(or to "escape") in order to distribute collision points. To avoid unnecessary tracking into regions of decreasing importance, we test, at each boundary, the integrand F(s) vs a fixed cutoff value F_0 (a number less than 1, which we like to set as 0.05). If, at some s_0, $F(s_0)$ becomes smaller than F_0, we Russian-roulette the remaining flight; with probability $[1-F(s_0)]$ we cut off the tracking, whereas with probability $F(s_0)$ we multiply the remaining density function F(s) by $1/F(s_0)$ and continue tracking. The case is illustrated in Figures Q.1c and Q.1d.

APPENDIX R

Procedure For Using Transmission Regions

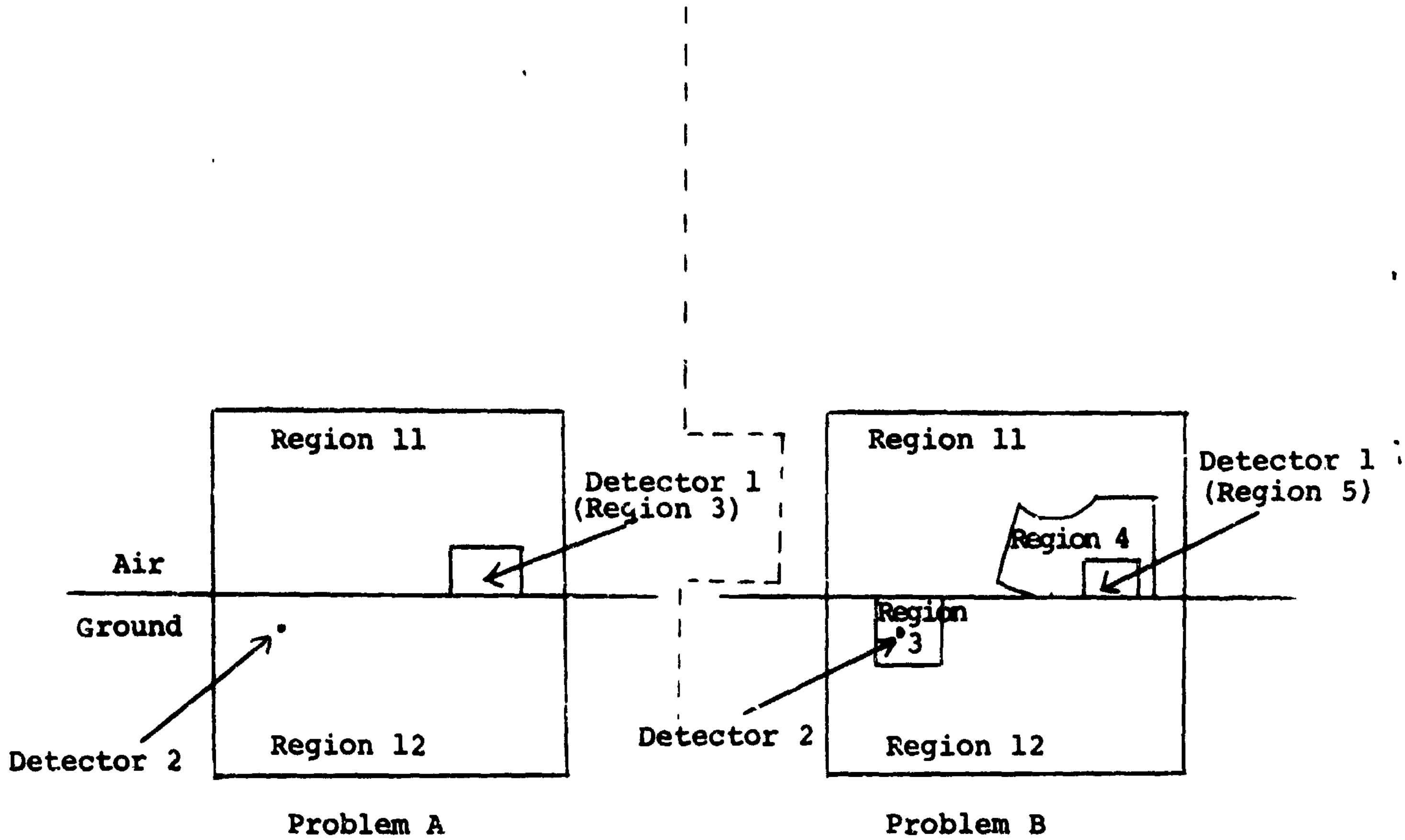
A transmission region would be used typically for problems where a portion of the geometry is subject to change, while the remainder of the problem (geometry and source) is constant, e.g., close calculations inside a variety of vehicles due to a weapon source in air. The following is a description of the procedures required to set up a particular problem.

1. General Procedure

Let problem A be that part of the total problem involving transport from the source to the transmission region (the source must be outside), and problem B that part involving transport through the transmission region.

In setting up problem A, describe the source according to 3.4.1. The geometry outside the transmission region(s) must be complete. The transmission regions themselves are considered as absorbers. However, separate regions must be used for each different composition at the interface with the real geometry (see Figure R.1, where regions labeled 11 and 12 are transmission regions.) Furthermore, if there are any detectors inside the transmission regions, these must be specified. Finally, any regions associated with small volume detectors must also be specified. The transmission data output will be on tape 14.

Problem B is set up as follows: the tape produced by problem A is labeled tape 15. The external source option (NSR=0) is used. The geometry must be complete, i.e., the true geometry of the transmission regions as well as the physical geometry of the



NOTE: Detector numbers (1 or 2) correspond.

Interface regions (11 or 12) correspond.

Small volume region (A-3,B-5) has same size and shape.

Point detector coordinates correspond.

Typical Transmission Region Geometry

Figure R.1

rest of problem A must be given. Finally, all detectors must be described.

In order that problem A and problem B match, the following correspondences must be made (see Figure R.1).

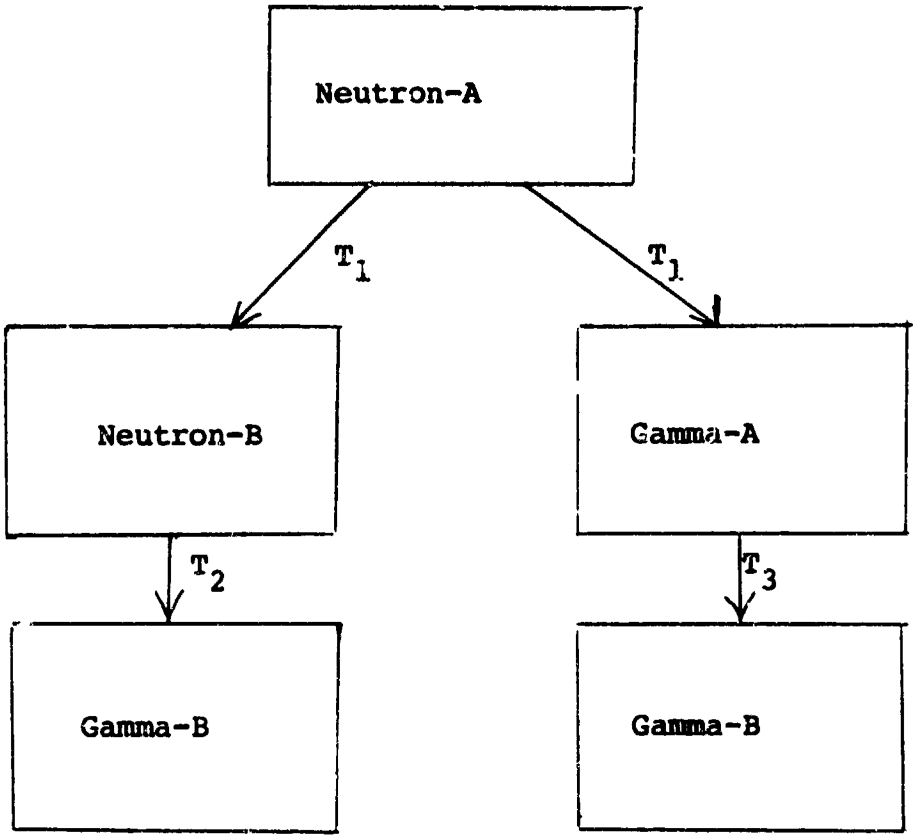
a. All detectors in the transmission regions must have the same identifying number (determined by the order of the input cards). Specifically, do not omit any detectors from problem B that are outside the transmission region.

b. The region numbers of the interfacing regions in problem B (determined by position in the region description deck) must be the same as the transmission regions of problem A.

c. The geometry of small volume detector regions must be the same in both problems, although the region numbers do not have to be the same. However (see (a)) the detector numbers must correspond.

2. Secondary Gammas

When secondary gammas are run with transmission regions, five passes are required, (1) neutron-A, (2) gamma-A, (3) neutron-B, (4 and 5) gamma-B (twice) where (2) and (3) may be interchanged. Figure R.2 is a schematic of the order. To get the complete answer, simply add the outputs of the two gamma-B runs. Note that the tape 14 produced by the neutron-A run is used as tape 15 for the gamma-A and neutron-B runs (NSR<0,NSR=0 respectively).



Each tape is labeled 14 as output and 15 as input.

T_1 contains both interactions and transmissions

T_2 contains only interactions.

T_3 contains only transmissions.

Secondary Gammas with Transmission Region

Figure R.2

APPENDIX S

Calculation of Dose by the Adjoint Monte Carlo Method

Consider the problem of calculating the dose at a detector within some shielding geometry due to a gamma ray source incident upon a geometry surface. Actual specification of the source distribution is given in terms of flux per energy and polar angle cosine bins. The polar angles are taken relative to the source-to-detector-axis. The subsequent discussion is directed toward finding the dose at the detector due to an elevated ring source rather than the point source for which the fluxes are specified. Presently, doses due to a point source, per se, can be calculated by the adjoint current option of SAM-A only for geometry with azimuthal symmetry. In the future it is expected to change the code so that this restriction will no longer hold true.

The approach adopted has been to separate the problem into two parts:

1) Utilization of the gamma ray adjoint Monte Carlo code SAM-A to calculate the adjoint current at the geometry outer surface for each detector point.
2) Folding the adjoint current with a given source distribution specified as a flux in energy-angle bins.

We now examine this problem quantitatively.

1. Theory

Consider first the angular variables involved in our problem by examining the unit sphere shown in Figure S.1a. Each point on the ring source is described by a unit vector (in the detector-to-source direction) $\vec{\Omega}_o$ where

$$\vec{\Omega}_o = (\sin\theta_o \cos\phi_o, \sin\theta_o \sin\phi_o, \cos\theta_o) \qquad \text{(S-1)}$$

Similarly another point on the sphere at which source fluxes and adjoint currents are specified is defined by a vector

$$\vec{\Omega} = \vec{\Omega}(\theta, \phi)$$

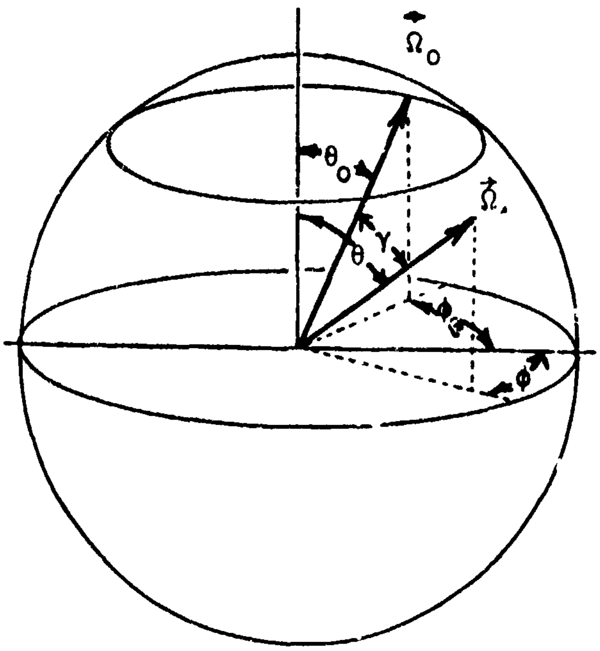


Figure S.1a. Angular Variables for the Ring and Source Points on a Unit Sphere. Angle θ_0 is the 60^o Angle of the Elevated Ring Source with the Vertical Direction.

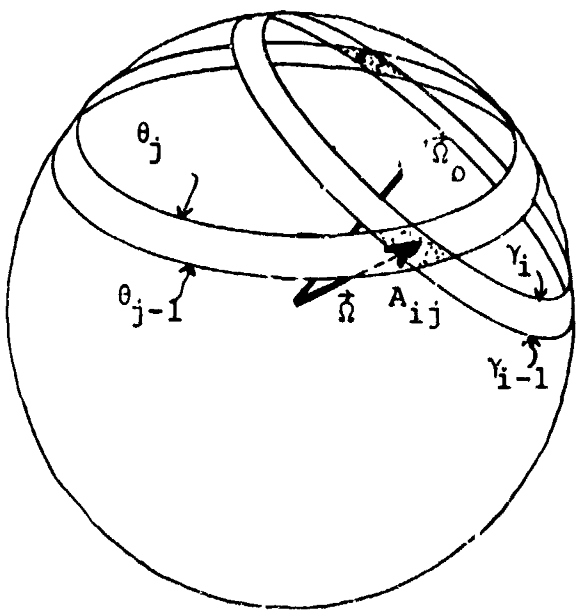


Figure S.1b. The Overlap Area A_{ij} on a Unit Sphere for $\vec{\Omega}_0$ Fixed (i.e., a Point Source). Rotation of $\vec{\Omega}_0$ about the Vertical Axis leaves A_{ij} Unchanged.

The adjoint current $J=J(\cos\theta,E)$ and the source flux $S=S(\cos\gamma,E)$ are specified in cosine-energy bins. S is assumed to be a constant S_{ik}, in a cosine bin $\cos\gamma_{i-1}-\cos\gamma_i$ and an energy bin $E_{k-1}-E_k$. Similarly J is a constant, J_{jk}, in bins of $\cos\theta_j$ and E_k.

The relationship between γ and θ,ϕ is given by

$$\cos\gamma = \cos\theta \cos\theta_o + \sin\theta \sin\theta_o \cos(\phi-\phi_o) \tag{S-2}$$

We first consider the dose $f(\vec{\Omega}_o)$ at the detector due to a point source having an angular orientation specified by $\vec{\Omega}_o$. As shown in reference 1, a flux functional such as the dose may be given in terms of a source term s(P) and an adjoint current term j(P)

as
$$f = \int j(P)\ s(P)dP \tag{S-3}$$

where

$$P = (\vec{r},E,\vec{\Omega})$$

for position, energy, and direction of photon.

It will be noted that in our case s(P)=S and that the dependence of S on $\cos\gamma$ may be specified in terms of $\vec{\Omega}$ and $\vec{\Omega}_o$ via Equation (S-2)Integration over $\vec{r}$ and ϕ is done (for j) within SAM-A. Furthermore, integration over $\cos\theta$ and E is performed in SAM-A for j within each of the specified bins.

Assuming integration over position variables has already been carried out, Equation (S-3) becomes

$$f(\vec{\Omega}_o) = \int S(\gamma\ (\theta,\phi,\theta_o,\phi_o),E)j(\theta,\phi,E)d(\cos\theta)d\phi dE \tag{S-4}$$

where the implicit dependence of γ on $\theta,\phi,\theta_o,\phi_o$ is exhibited.

The average over the elevated ring source is now easily obtained. It is given by

$$F = \int_0^{2\pi} f(\vec{\Omega}_o) \frac{d\phi_o}{2\pi} \tag{S-5}$$

Equation (S-2) shows that if we define

$$\beta = \phi - \phi_o \tag{S-6}$$

then the functional dependence of γ is given by

$$\gamma = \gamma(\theta, \beta, \theta_o) \tag{S-7}$$

Utilizing Equations S-2 to S-7 allows us to write

$$F = \int_{E_L}^{E_H} dE \int_{-1}^{1} d(\cos\theta) \int_0^{2\pi} d\beta \quad S(\gamma(\theta,\beta,\theta_o),E) \quad J(\theta,E) \tag{S-8}$$

where

$$J(\theta,E) = \int_0^{2\pi} j(\theta,\phi,E) \frac{d\phi}{2\pi} \tag{S-9}$$

Equation (S-9) expresses the fact that the integration over ϕ may be carried out for J prior to integration over the other variables and is indeed carried out within SAM-A as mentioned above. For S and J specified in the energy-polar cosine bins defined above, Equation (S-8) reduces to

$$F = \sum_{ijk} S_{ik} \; J_{jk} \; A_{ij} \tag{S-10}$$

where

$$A_{ij} = \int_{\cos\theta_{j-1}}^{\cos\theta_j} d(\cos\theta) \int_{\beta_{i-1}}^{\beta_i} d\beta \qquad \text{(S-11)}$$

A little thought will show that A_{ij} is just the overlap of the θ and solid angle polar cosine bands shown in Figure S.1b. A_{ij} can be evaluated either by numerical integration or analytically by the use of theorems from spherical geometry . Numerical integration involves the following considerations:

Equation (S-2) may be rewritten as:

$$\beta = \text{Arc}\cos\left(\frac{x - \cos\theta\cos\theta_o}{\sin\theta\sin\theta_o}\right), \quad x = \cos\gamma \qquad \text{(S-12)}$$

We are left with a final expression

$$F = 2\sum_{ijk} S_{ik} J_{jk} \int_{\cos\theta_{j-1}}^{\cos\theta_j} d(\cos\theta)\ \text{Arc}\cos\left(\frac{x - \cos\theta\cos\theta_o}{\sin\theta\sin\theta_o}\right)\Bigg|_{x=x_{i-1}}^{x=x_i} \qquad \text{(S-13)}$$

where the factor 2 comes from the fact that β in Equation (S-12) is doubly defined.

The argument of Arc cos sets limits on the allowed values of $\cos\theta$ which may be shown to be:

$$x\cos\theta_o - \sqrt{1-x^2}\sin\theta_o \leq \cos\theta \leq x\cos\theta_o + \sqrt{1-x^2}\sin\theta_o \qquad \text{(S-14)}$$

or alternatively the condition on x becomes:

$$\cos(\theta+\theta_o) \leq x \leq \cos(\theta-\theta_o) \qquad \text{(S-15)}$$

These conditions define the interior of an ellipse in the plane defined by an abscissa x and an ordinate $\cos\theta$ with the semi-major axis pointing along an angle of $\pi/4$ radians with respect to either the x or $\cos\theta$ axis.

Note that Equation (S-13) may be written as the matrix expression:

$$F = \mathrm{Tr}\left[(SJ)A)\right] \qquad \text{(S-16)}$$

so that for a given set of angular bins the matrix A need be calculated only once and the summation over ijk is then performed for each different building-detector configuration.

A discussion of the units and normalizations required to give the correct dose follows.

2. An Example of the Uses of Units and Normalizations

Let us return to the basic Equations (S-10), (S-11) to consider the units and normalizations we must use. J_{jk} represents the adjoint current i.e., the total number of particles crossing a particular surface in a particular energy-polar cosine bin. It is calculated in SAM-A. To see what it represents consider the simple problem of a point detector surrounded by a surface an epsilon distance from the point. SAM-A then yields a quantity which is proportional to the response function (a function of energy only) at the detector in each energy-cosine bin. Indeed the calculated quantity is

$$J_{jk} = R_k/\ \Delta\cos\theta_j/(2/\Delta\cos\theta_j)$$

$$= R_k/2. \qquad \text{(S-17)}$$

Let us consider an example in which the response function is given in units of (rads/hr)/(photons/cm^2-sec). Assume the S_{ik} are given as the source flux in units of (photons/Mev-steradian-source neutron). To obtain the proper energy relationship it is then necessary to multiply Equation (S-17) by ΔE_k. As far as solid angle is concerned the A_{ij} themselves are the proper normalization factor. However, since in the edit, the normalization $\sum_i A_{ij} = 1$ is used, a factor of 4π is necessary. A factor of 2 is necessary from Equation (S-17) and division by 3600 is required to make the response function independent of time. The total multiplication factor required for secondary gamma rays is

$$f_s = (4\pi)(2)/(3600) = 0.698\text{X}10^{-2}\ , \qquad \text{(S-18)}$$

and Equation (S-10) yields the free field dose

$$F_{fs} = f_s \sum_{ijk} \Delta E_k \frac{R_k}{2} S_{ik} A_{ij} \text{ rads-cm}^2\text{/source neutron.} \quad (S-19)$$

For the non-free field case one replaces R_k by J_{jk} in Equation (S-19).

REFERENCE FOR APPENDIX S

1. M. H. Kalos, "Monte Carlo Integration of the Adjoint Gamma-Ray Transport Equation", Nuc. Sci. & Eng., 33, 284-290 (1968).

SECTION 6: INDEX (BY PROGRAM)

PROGRAM SAM-X

PROGRAM SAM-F

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PROGRAM SAM-F (Continued)

PROGRAM SAM-A